Full wwPDB EM Validation Report ⓘ

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PDB ID	:	8JXI
EMDB ID	:	EMD-36702
Title	:	rat megalin RAP complex wingB
Authors	:	Goto, S.; Tsutsumi, A.; Lee, Y.; Hosojima, M.; Kabasawa, H.; Komochi, K.; Yun-san, L.; Nagatoshi, S.; Tsumoto, K.; Nishizawa, T.; Kikkawa, M.; Saito, A.
Deposited on	:	2023-06-30
Resolution	:	3.40 Å(reported)
Based on initial model	:	.

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

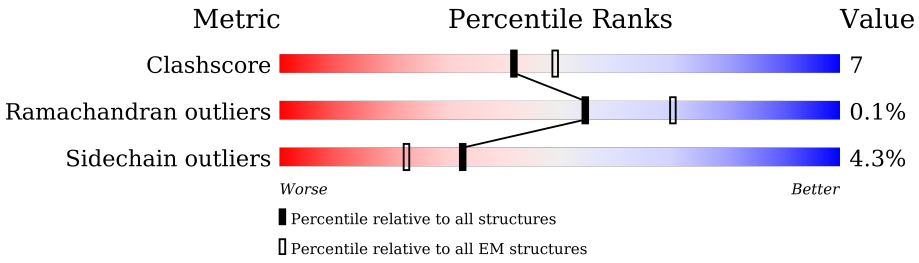
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	332	10% 23% 8% 68%
2	A	4660	21% 75%
2	B	4660	97%
3	G	6	100%
4	H	5	100%
5	D	2	50% 100%
5	I	2	50% 100%
6	E	5	40% 60% 40%

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Mol	Chain	Length	Quality of chain
7	F	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	A2G	A	4705	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11506 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Alpha-2-macroglobulin receptor-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	C	105	Total	C	N	O	0	0
			895	563	163	169		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	GLY	-	expression tag	UNP Q99068
C	30	PRO	-	expression tag	UNP Q99068
C	31	LEU	-	expression tag	UNP Q99068
C	32	GLY	-	expression tag	UNP Q99068
C	33	SER	-	expression tag	UNP Q99068

- Molecule 2 is a protein called LDL receptor related protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	1167	Total	C	N	O	S	0	0
			9053	5548	1609	1788	108		
2	B	148	Total	C	N	O	S	0	0
			1124	665	197	241	21		

- Molecule 3 is a protein called unclear peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	6	Total	C	N	O	0	0
			30	18	6	6		

- Molecule 4 is a protein called unclear peptide.

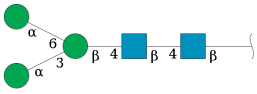
Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	5	Total	C	N	O	0	0
			28	16	6	6		

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a

cetamido-2-deoxy-beta-D-glucopyranose.

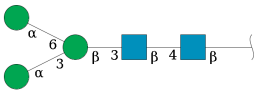
Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	2	Total	C	N	O	0	0
			28	16	2	10		
5	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



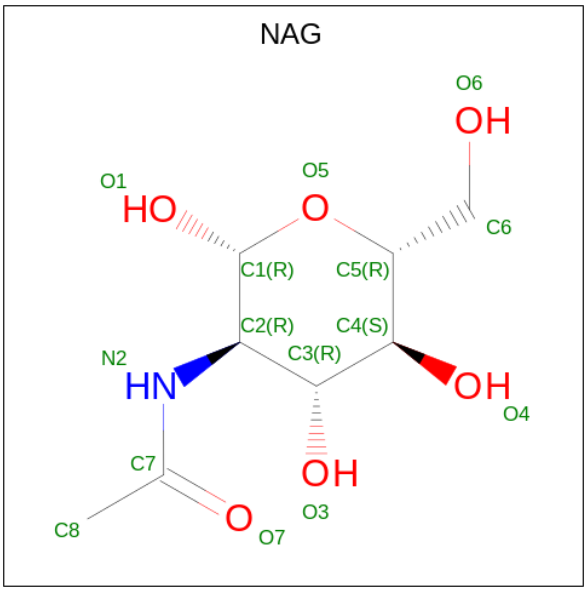
Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



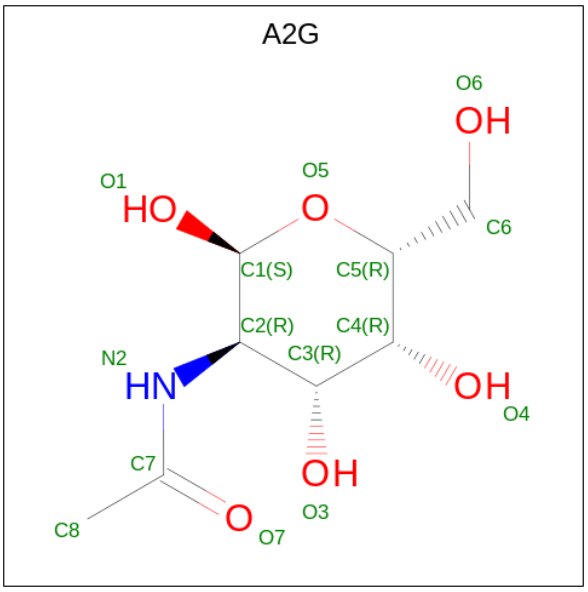
Mol	Chain	Residues	Atoms				AltConf	Trace
7	F	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
8	A	1	Total C N O 14 8 1 5	0
8	A	1	Total C N O 14 8 1 5	0
8	B	1	Total C N O 14 8 1 5	0
8	B	1	Total C N O 14 8 1 5	0

- Molecule 9 is 2-acetamido-2-deoxy-alpha-D-galactopyranose (three-letter code: A2G) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
9	A	1	Total 14	C 8	N 1	O 5	0
9	A	1	Total 14	C 8	N 1	O 5	0
9	A	1	Total 14	C 8	N 1	O 5	0
9	A	1	Total 14	C 8	N 1	O 5	0
9	A	1	Total 14	C 8	N 1	O 5	0
9	A	1	Total 14	C 8	N 1	O 5	0
9	A	1	Total 14	C 8	N 1	O 5	0
9	A	1	Total 14	C 8	N 1	O 5	0
9	B	1	Total 14	C 8	N 1	O 5	0

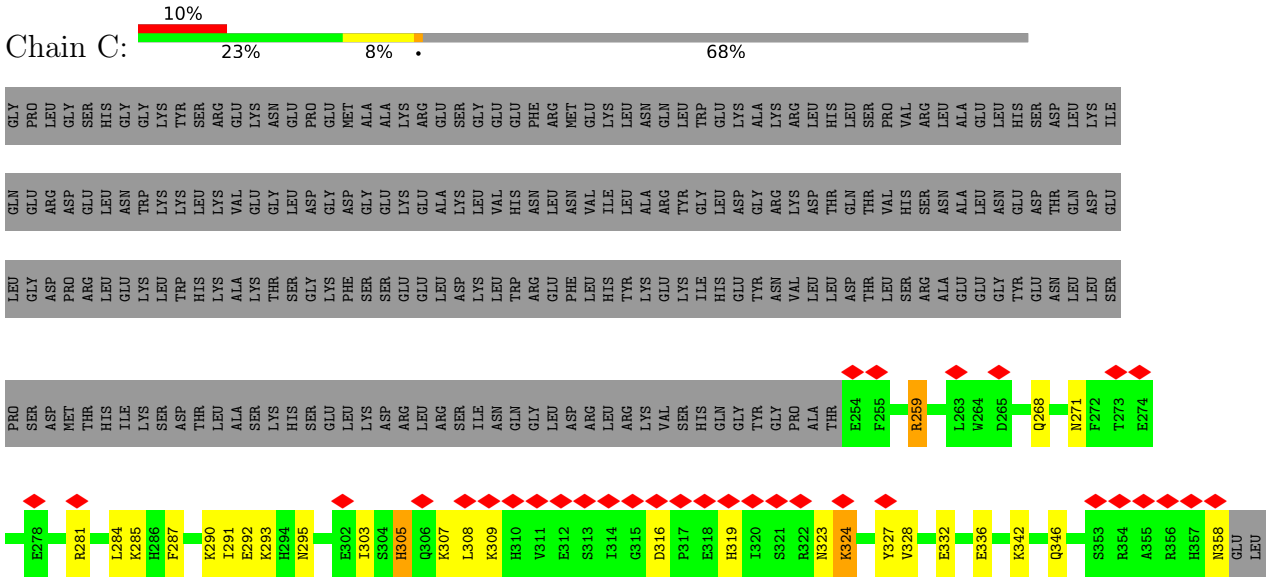
- Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
10	A	12	Total 12	Ca 12	0
10	B	4	Total 4	Ca 4	0

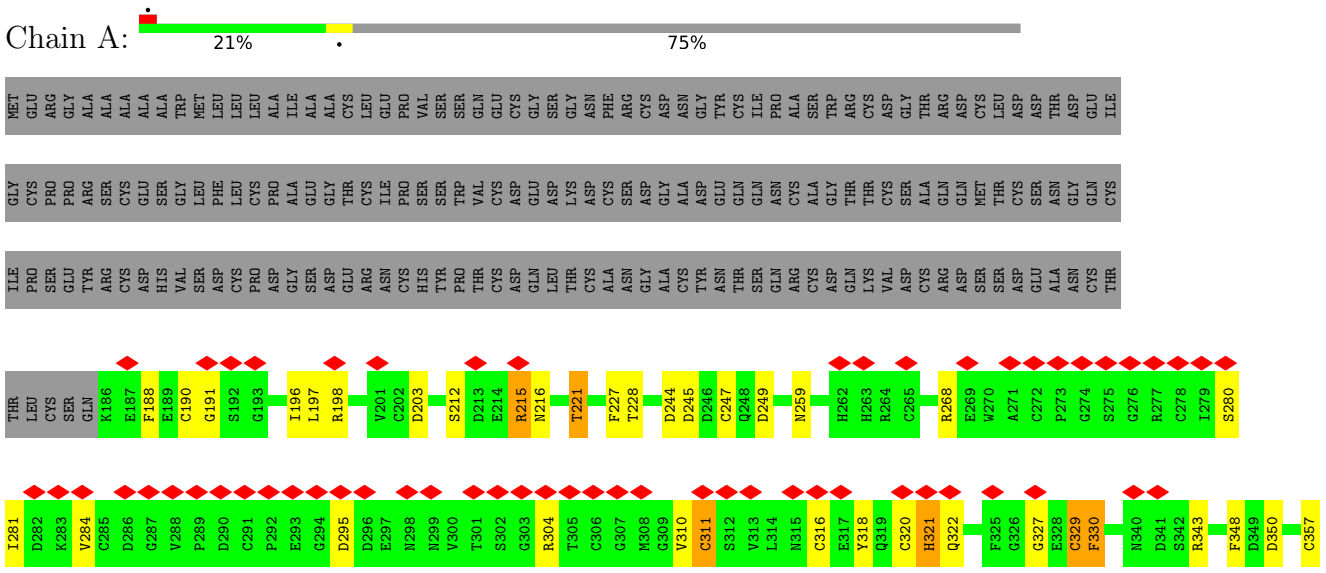
3 Residue-property plots (i)

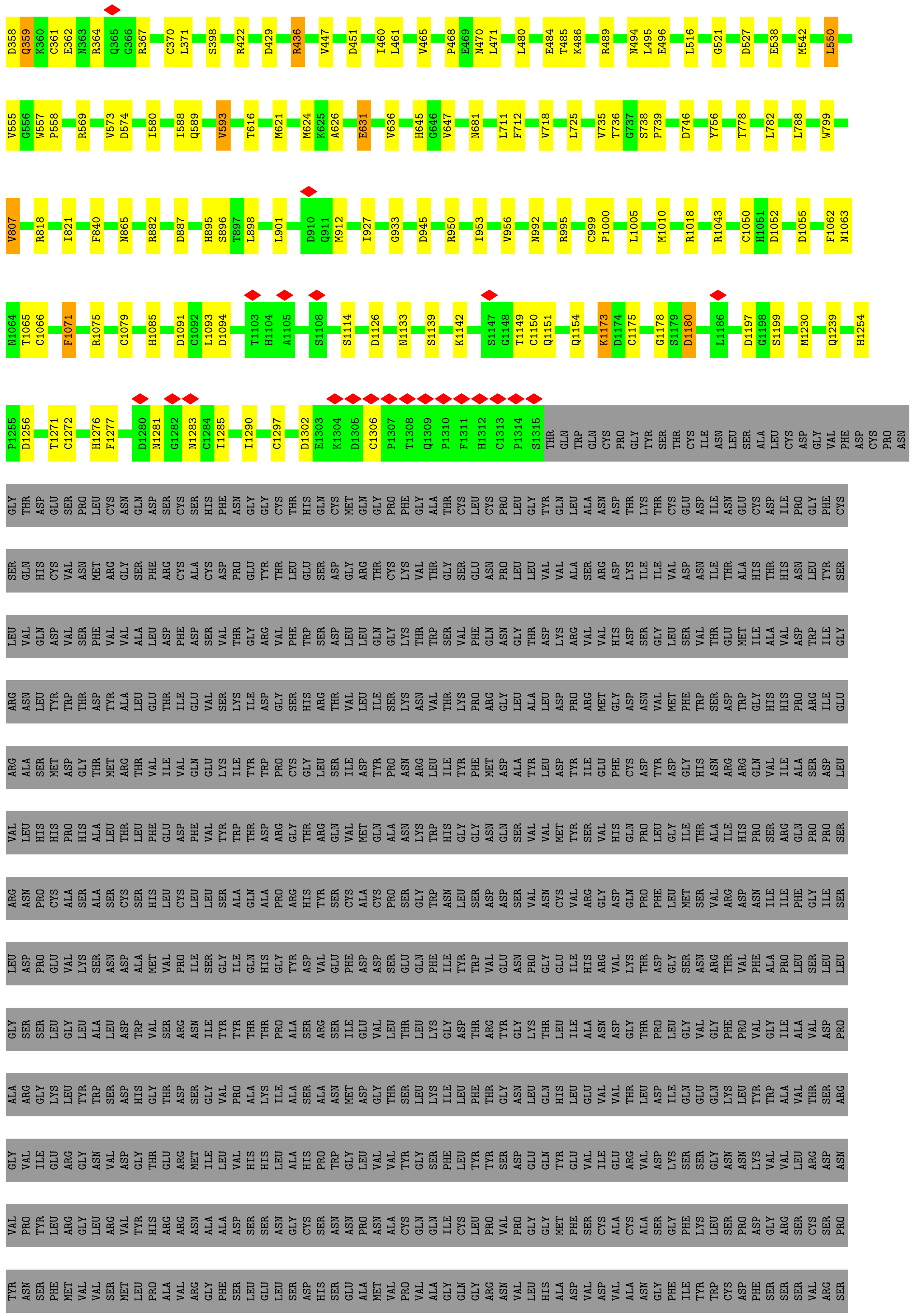
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Alpha-2-macroglobulin receptor-associated protein



• Molecule 2: LDL receptor related protein 2

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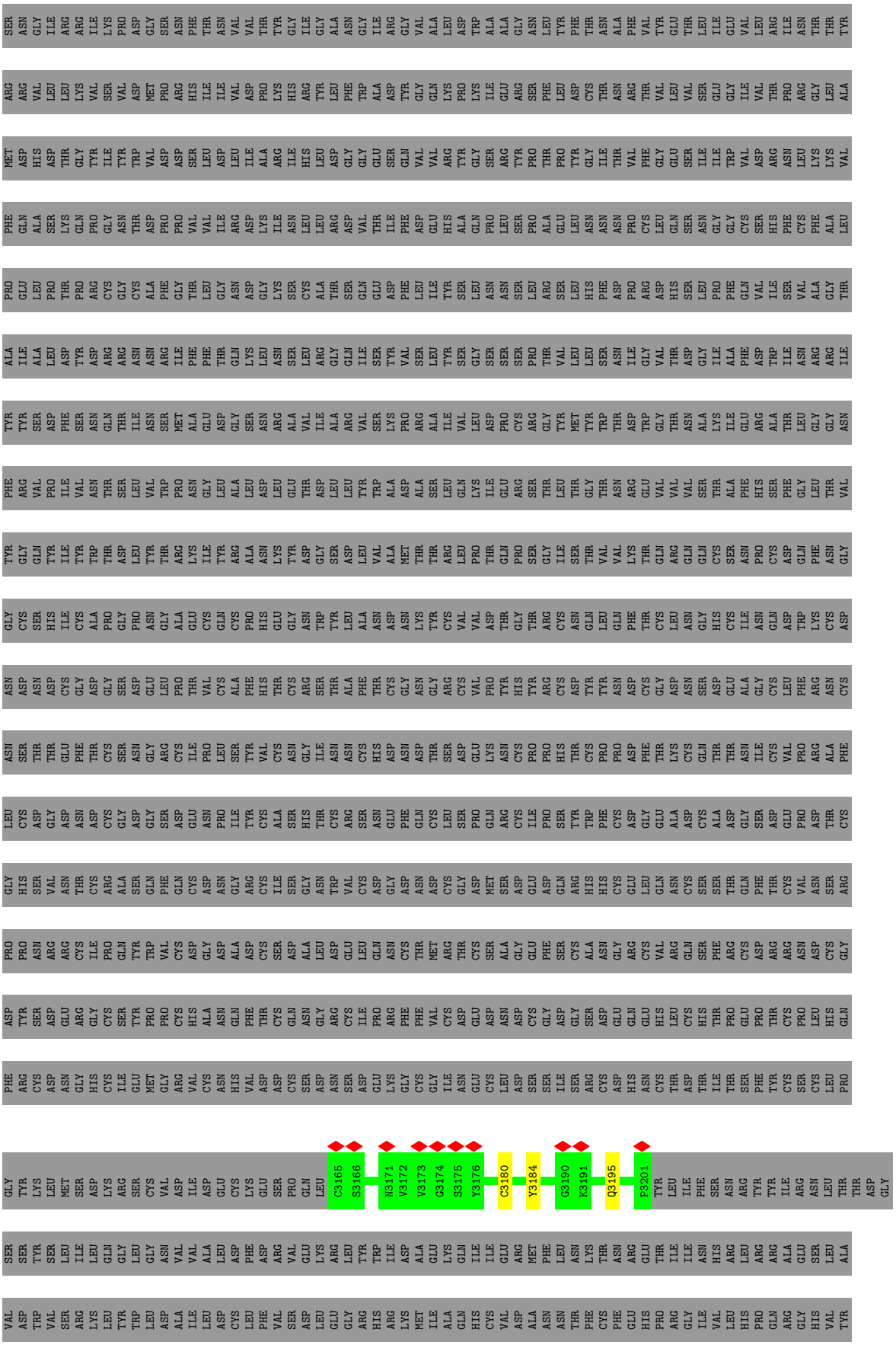
V555 G556 W557 P558 R569 V573 D574 I580 I588 Q589 V593 T616 M621 M624 K625 A626 E631 V636 H645 G646 V647 N681 L711 F712 V718 L725 V735 T736 G737 S738 P739 D746 Y756 T778 L782 L788 W799
V807 R818 I821 F840 N865 R882 D887 H895 S896 T897 L898 L901 D910 Q911 M912 I927 G933 D945 R950 I953 V956 N992 R995 C999 P1000 L1005 M1010 R1018 R1043 C1050 H1051 D1052 D1055 F1062 N1063
N1064 T1065 C1066 F1071 R1075 C1079 H1085 D1091 C1092 L1093 D1094 T1103 H1104 A1105 S1108 S1114 D1126 N1133 S1139 K1142 S1147 G1148 T1149 C1150 Q1151 Q1154 K1173 D1174 C1175 G1178 S1179 D1180 L1186 D1197 G1198 S1199 M1230 Q1239 H1254
P1255 D1256 T1271 C1272 H1276 F1277 D1280 N1281 G1282 N1283 C1284 I1285 I1290 C1297 D1302 E1303 K1304 D1305 C1306 P1307 T1308 Q1309 P1310 F1311 H1312 C1313 P1314 S1315 THR GLN TRP GLN CYS PRO GLY TYR SER THR CYS ILE ASN LEU SER ALA LEU CYS ASP GLY VAL PHE ASP CYS PRO ASN
GLY THR ASP GLU SER PRO LEU CYS ASN GLN ASP SER CYS SER HIS PHE ASN GLY GLY CYS THR HIS GLN CYS MET GLN GLY PRO PHE GLY ALA THR CYS LEU CYS PRO LEU GLY TYR GLN LEU ALA ASN ASP THR LYS THR CYS GLU ASP ILE ASN GLU CYS ASP ILE PRO GLY PHE CYS
SER GLN HIS CYS VAL ASN MET ARG GLY SER PHE ARG CYS ALA CYS ASP PRO GLU TYR THR LEU GLU SER ASP GLY ARG THR CYS LYS VAL THR GLY SER GLU ASN PRO LEU LEU VAL VAL ALA SER ARG ASP LYS ILE ILE VAL ASP ASN ILE THR ALA HIS THR HIS ASN LEU TYR SER
LEU VAL GLN ASP VAL SER PHE VAL VAL ALA LEU ASP PHE ASP SER VAL THR GLY ARG VAL PHE TRP SER ASP LEU LEU GLN GLY LYS THR TRP SER VAL PHE GLN ASN GLY THR ASP LYS ARG VAL VAL HIS ASP SER GLY LEU SER VAL THR GLU MET ILE ALA VAL ASP TRP ILE GLY
ARG ASN LEU TYR TRP THR ASP TYR ALA LEU GLU THR ILE GLU VAL SER LYS ILE ASP GLY SER HIS ARG THR VAL LEU ILE SER LYS ASN VAL THR LYS PRO ARG GLY LEU ALA LEU ASP PRO ARG MET GLY ASP ASN VAL MET PHE TRP SER ASP TRP GLY HIS HIS PRO ARG ILE GLU
ARG ALA SER MET ASP GLY THR MET ARG THR VAL ILE VAL GLN GLU LYS ILE TYR TRP PRO CYS GLY LEU SER ILE ASP TYR PRO ASN ARG LEU ILE TYR PHE MET ASP ALA TYR LEU ASP TYR ILE GLU PHE CYS ASP TYR ASP GLY HIS ASN ARG ARG GLN VAL ILE ALA SER ASP LEU
VAL LEU HIS HIS PRO HIS ALA LEU THR LEU PHE GLU ASP PHE VAL TYR TRP THR ASP ARG GLY THR ARG GLN VAL MET GLN ALA ASN LYS TRP HIS GLY GLY ASN GLN SER VAL VAL MET TYR SER VAL HIS GLN PRO LEU GLY ILE THR ALA ILE HIS PRO SER ARG GLN PRO PRO SER
ARG ASN PRO CYS ALA SER ALA SER CYS SER HIS LEU CYS LEU LEU SER ALA GLN ALA PRO ARG HIS TYR SER CYS ALA CYS PRO SER GLY TRP ASN LEU SER ASP ASP SER VAL ASN CYS VAL ARG GLY ASP GLN PRO PHE LEU MET SER VAL ARG ASP ASN ILE ILE PHE GLY ILE SER
LEU ASP PRO GLU VAL LYS SER ASN ASP ALA MET VAL PRO ILE SER GLY ILE GLN HIS GLY TYR ASP VAL GLU PHE ASP ASP SER GLU GLN PHE ILE TYR TRP VAL GLU ASN PRO GLY GLU ILE HIS ARG VAL LYS THR ASP GLY SER ASN ARG THR VAL PHE ALA PRO LEU SER LEU LEU
GLY SER SER LEU GLY LEU ALA LEU ASP TRP VAL SER ARG ASN ILE TYR TYR THR THR PRO ALA SER ARG SER ILE GLU VAL LEU THR LEU LYS GLY ASP THR ARG TYR GLY LYS THR LEU ILE ALA ASN ASP GLY THR PRO LEU GLY VAL GLY PHE PRO VAL GLY ILE ALA VAL ASP PRO
ALA ARG GLY LYS LEU TYR TRP SER ASP HIS GLY THR ASP SER GLY VAL PRO ALA LYS ILE ALA SER ALA ASN MET ASP GLY THR SER LEU LYS ILE LEU PHE THR GLY ASN LEU GLN HIS LEU GLU VAL VAL THR LEU ASP ILE GLN GLU GLN LYS LEU TYR TRP ALA VAL THR SER ARG
GLY VAL ILE GLU ARG GLY ASN VAL ASP GLY THR GLU ARG MET ILE LEU VAL HIS HIS LEU ALA HIS PRO TRP GLY LEU VAL VAL TYR GLY SER PHE LEU TYR TYR SER ASP GLU GLN TYR GLU VAL ILE GLU ARG VAL ASP LYS SER SER GLY ASN ASN LYS VAL VAL LEU ARG ASP ASN
VAL PRO TYR LEU ARG GLY LEU ARG VAL TYR HIS ARG ARG ASN ALA ALA ASP SER SER ASN GLY CYS SER ASN ASN PRO ASN ALA CYS GLN GLN ILE CYS LEU PRO VAL PRO GLY GLY MET PHE SER CYS ALA CYS ALA SER GLY PHE LYS LEU SER PRO ASP GLY ARG SER CYS SER PRO
TYR ASN SER PHE MET VAL VAL SER MET LEU PRO ALA VAL ARG GLY PHE SER LEU GLU LEU SER ASP HIS SER GLU ALA MET VAL PRO VAL ALA GLY GLN GLY ARG ASN VAL LEU HIS ALA ASP VAL ASP VAL ALA ASN GLY PHE ILE TYR TRP CYS ASP PHE SER SER SER VAL ARG SER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S3166
N3171
V3172
V3173
G3174
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Y3176
C3180
Y3184
G3190
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Q3195
P3201

TRP ALA ASP TRP GLY VAL HIS ALA TYR ILE GLY ARG ILE GLY MET ASP GLY THR ASN LYS SER VAL ILE ILE SER THR LYS ILE GLU TRP PRO ASN ALA ILE THR ILE ASP TYR THR ASN ASP LEU LEU TYR TRP ALA ASP ALA HIS LEU GLY TYR ILE GLU PHE SER ASP LEU GLU GLY

HIS HIS ARG HIS THR VAL TYR ASP GLY SER LEU PRO HIS PRO PHE ALA LEU THR ILE PHE GLU ASP THR VAL PHE TRP THR ASP TRP ASN THR ARG THR VAL GLU LYS GLY ASN LYS TYR ASP GLY SER GLY ARG VAL VAL LEU VAL ASN THR THR HIS LYS PRO PHE ASP ILE HIS VAL

TYR HIS PRO TYR ARG GLN PRO ILE MET SER ASN PRO CYS GLY THR ASN ASN GLY GLY CYS SER HIS LEU CYS LEU ILE LYS ALA GLY GLY ARG GLY PHE THR CYS ALA CYS PRO ASP ASP PHE GLN THR VAL GLN LEU ARG ASP ARG THR LEU CYS MET PRO MET CYS SER SER THR GLN

PHE LEU CYS GLY ASN ASN GLU LYS CYS ILE PRO ILE TRP TRP LYS CYS ASP GLY GLN LYS ASP CYS SER ASP GLY SER ASP GLU PRO ASP LEU CYS PRO HIS ARG PHE CYS ARG LEU GLY GLN PHE GLN CYS ARG ASP GLY ASN CYS THR SER PRO GLN ALA LEU CYS ASN ALA ARG GLN

ASP CYS ALA ASP GLY SER ASP GLU ASP ARG VAL LEU CYS GLU HIS HIS ARG CYS GLU SER ASN GLU TRP GLN CYS ALA ASN LYS ARG CYS ILE PRO GLN SER TRP GLN CYS ASP SER SER VAL ASN ASP CYS LEU ASP ASN SER ASP GLU ASP THR SER HIS CYS ALA SER ARG THR CYS ARG

PRO GLY GLN PHE LYS CYS ASN ASN GLY ARG CYS ILE PRO GLN SER TRP LYS CYS ASP VAL ASP ASN ASP CYS GLY ASP TYR SER ASP GLU PRO ILE ASP GLU CYS THR THR ALA ALA TYR ASN CYS ASP ASN HIS THR GLU PHE SER CYS LYS THR ASN TYR ARG CYS ILE PRO GLN TRP

ALA VAL CYS ASN GLY PHE ASP ASP CYS ARG ASP ASN SER ASP GLU GLN GLY CYS GLU SER VAL PRO CYS HIS PRO SER GLY ASP PHE ARG CYS ALA ASN HIS HIS CYS ILE PRO LEU ARG TRP LYS CYS ASP GLY THR ASP ASP CYS GLY ASP ASN SER ASP GLU GLU ASN CYS VAL PRO

ARG GLU CYS SER GLU SER GLU PHE ARG CYS ALA ASP GLN GLN CYS ILE PRO SER ARG TRP VAL CYS ASP GLN GLU ASN ASP CYS GLY ASP ASN SER ASP GLU ARG ASP CYS GLU MET LYS THR CYS HIS PRO GLU HIS PHE GLN CYS THR SER GLY HIS CYS VAL PRO LYS ALA LEU ALA

CYS ASP GLY ARG ALA ASP CYS LEU ASP ALA SER ASP GLU SER ALA CYS PRO THR ARG PHE PRO ASN GLY THR TYR CYS PRO ALA ALA MET PHE GLU CYS LYS ASN HIS VAL CYS ILE GLN SER PHE TRP ILE CYS ASP GLY GLU ASN ASP CYS VAL ASP GLY SER ASP GLU GLU ILE HIS

LEU CYS PHE ASN ILE PRO CYS GLU SER PRO GLN ARG PHE ARG CYS ASP ASN SER ARG CYS VAL TYR GLY HIS GLN LEU CYS ASN GLY VAL ASP ASP CYS GLY ASP GLY SER ASP GLU LYS GLU GLU HIS CYS ARG LYS PRO THR HIS LYS PRO CYS THR ASP THR GLU TYR LYS CYS SER

ASN GLY ASN CYS ILE SER GLN HIS TYR VAL CYS ASP ASN VAL ASN ASP CYS GLY ASP LEU SER ASP GLU THR GLY CYS ASN LEU GLY ASP ASN ARG THR CYS ALA GLU ASN ILE CYS GLU GLN ASN CYS THR GLN LEU SER SER GLY GLY PHE ILE CYS SER CYS ARG PRO GLY PHE LYS

PRO SER THR LEU ASP LYS ASN SER CYS GLN ASP ILE ASN GLU CYS GLU GLU PHE GLY ILE CYS PRO GLN SER CYS ARG ASN SER LYS GLY SER TYR GLU CYS PHE CYS VAL ASP GLY PHE LYS SER MET SER THR HIS TYR GLY GLU ARG CYS ALA ALA ASP GLY SER PRO PRO LEU LEU

LEU LEU PRO GLU ASN VAL ARG ILE ARG LYS TYR ASN THR SER SER GLU LYS PHE SER GLU TYR LEU GLU GLU GLU GLU HIS ILE GLN THR ILE ASP TYR ASP TRP ASP PRO GLU HIS ILE GLY LEU SER VAL VAL TYR TYR THR VAL LEU ALA GLN GLY SER GLN PHE GLY ALA ILE LYS

ARG ALA TYR ILE PRO ASN PHE GLU SER GLY SER ASN ASN PRO ILE ARG GLU VAL ASP LEU GLY LEU LYS TYR LEU MET GLN PRO ASP GLY LEU ALA VAL ASP TRP VAL GLY ARG HIS ILE TYR TRP SER ASP ALA LYS SER GLN ARG ILE GLU VAL ALA THR LEU ASP GLY ARG TYR ARG

LYS TRP LEU ILE THR THR GLN LEU ASP GLN PRO ALA ALA ILE ALA VAL ASN PRO LYS LEU GLY LEU MET PHE TRP THR ASP GLN GLY LYS GLN PRO LYS ILE GLU SER ALA TRP MET ASN GLY GLU HIS ARG SER VAL LEU VAL SER GLU ASN LEU GLY TRP PRO ASN GLY LEU SER ILE

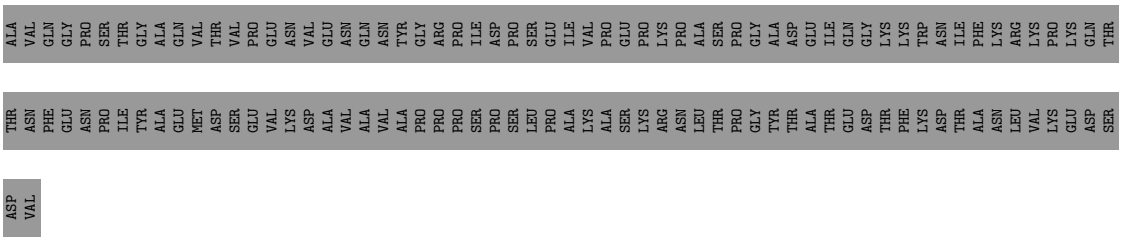
ASP TYR LEU ASN ASP ASP ARG VAL TYR TRP SER ASP SER LYS GLU ASP VAL ILE GLU ALA ILE LYS TYR ASP GLY THR ASP ARG ARG LEU ILE ILE ASN GLU ALA MET LYS PRO PHE SER LEU ASP ILE PHE GLU ASP LYS LEU TYR TRP VAL ALA LYS GLU LYS GLY GLU VAL TRP ARG

GLN ASN LYS PHE GLY LYS GLU ASN LYS GLU LYS VAL LEU VAL VAL ASN PRO TRP LEU THR GLN VAL ARG ILE PHE HIS GLN LEU ARG TYR ASN GLN SER VAL SER ASN PRO CYS LYS GLN VAL CYS SER HIS LEU CYS LEU LEU ARG PRO GLY GLY TYR SER CYS ALA CYS PRO GLN GLY

SER ASP PHE VAL THR GLY SER THR VAL GLN CYS ASP ALA ALA SER GLU LEU PRO VAL THR MET PRO PRO PRO CYS ARG CYS MET HIS GLY GLY ASN CYS TYR PHE ASP GLU ASN GLU LEU PRO LYS CYS LYS CYS SER SER GLY TYR SER GLY GLU TYR CYS GLU VAL GLY LEU SER ARG

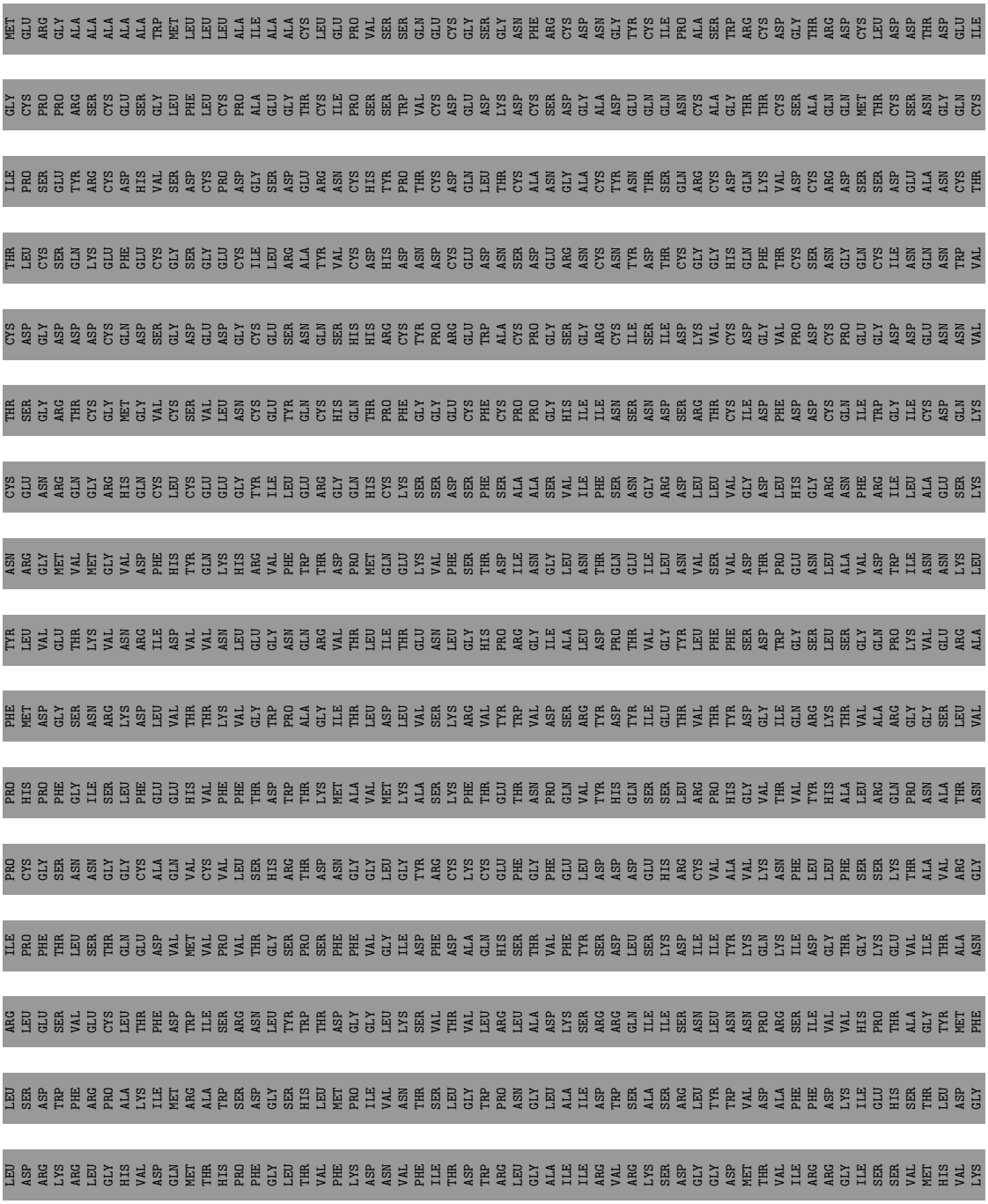
GLY ILE PRO PRO GLY THR THR MET ALA VAL LEU LEU THR PHE VAL ILE VAL ILE ILE VAL GLY ALA LEU VAL LEU VAL GLY LEU PHE HIS TYR ARG LYS THR GLY SER LEU LEU PRO THR LEU PRO LYS LEU PRO SER LEU SER SER LEU ALA LYS PRO SER GLU ASN GLY ASN GLY VAL

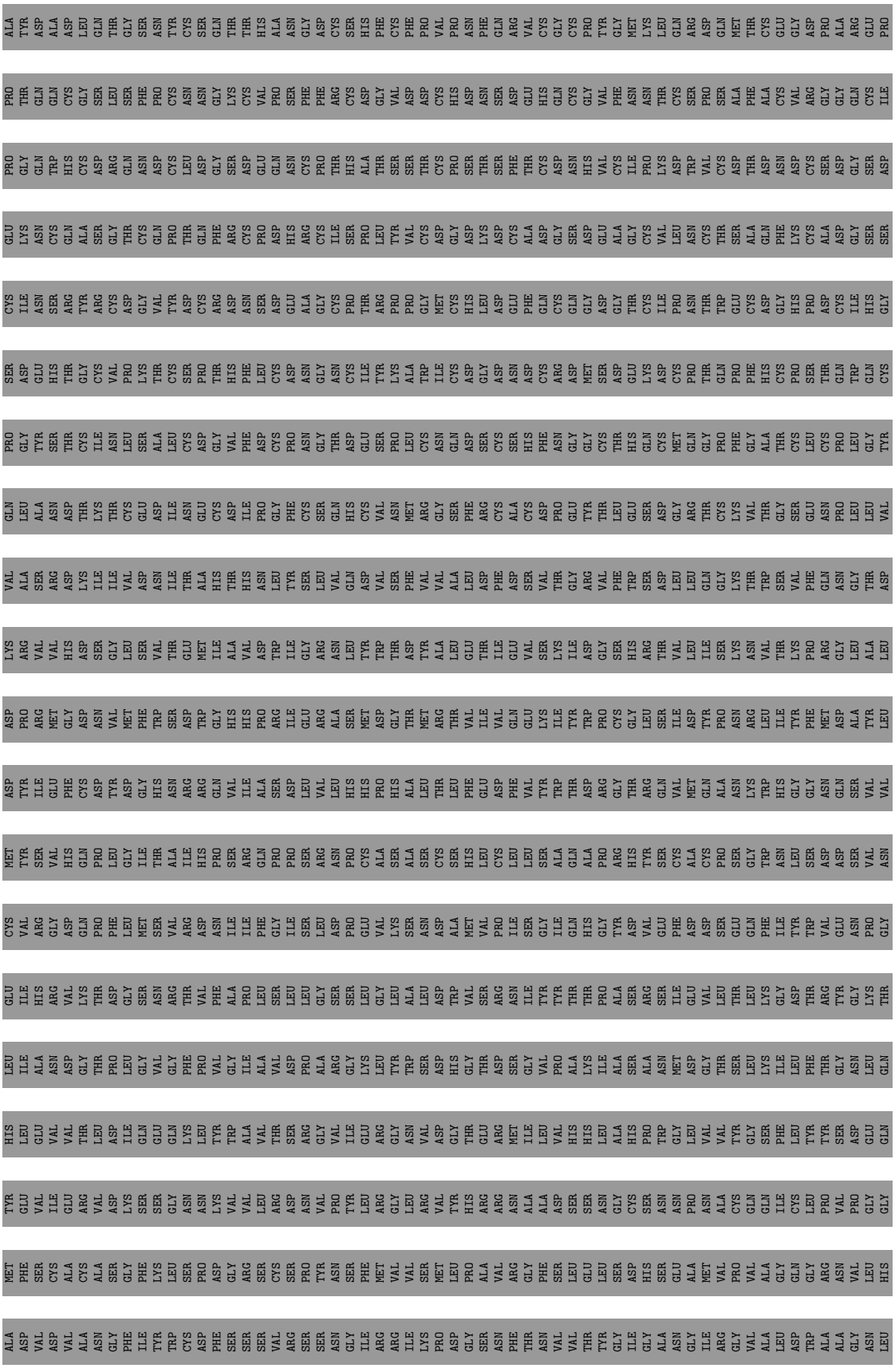
THR PHE ARG SER GLY ALA ASP VAL ASN MET ASP ILE GLY VAL SER PRO PHE GLY PRO GLU THR ILE ILE ASP ARG SER MET ALA MET ASN GLU HIS PHE VAL MET GLU VAL GLY LYS GLN PRO VAL ILE PHE GLU ASN PRO MET TYR ALA ALA LYS ASP ASN THR SER LYS VAL ALA LEU

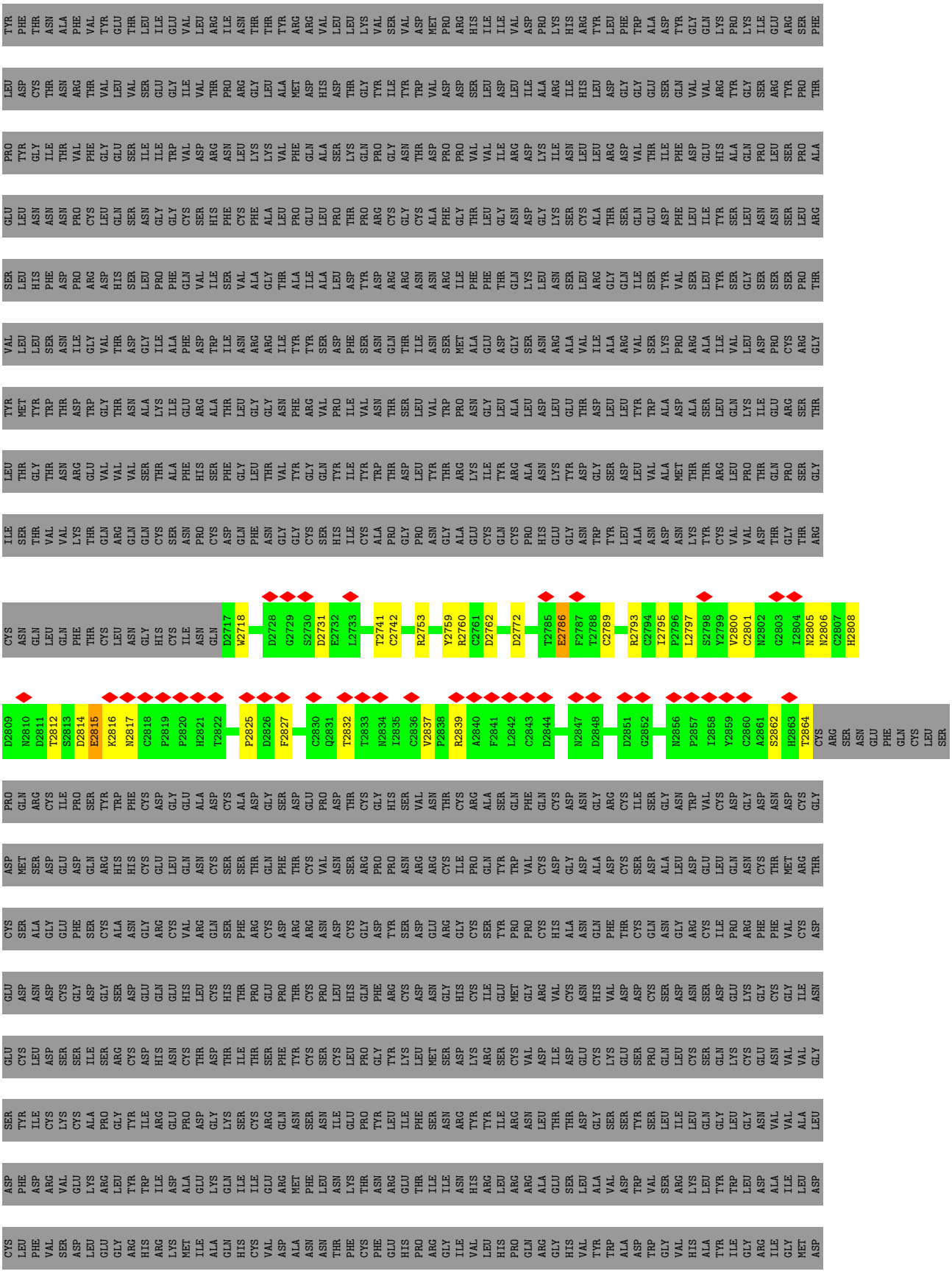


• Molecule 2: LDL receptor related protein 2

Chain B: 97%





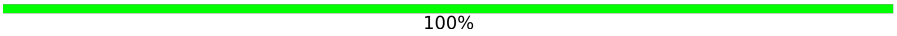


VAL GLU ASN GLN ASN TYR GLY ARG PRO ILE ASP PRO SER GLU ILE VAL PRO GLU PRO LYS PRO ALA SER PRO GLY ALA ASP GLU ILE GLN GLY LYS LYS TRP ASN ILE PHE LYS ARG LYS PRO LYS GLN THR THR ASN PHE GLU ASN PRO ILE TYR ALA GLU MET ASP SER GLU VAL LYS

ASP ALA VAL ALA VAL ALA PRO PRO PRO SER PRO SER LEU PRO ALA LYS ALA SER LYS ARG ASN LEU THR PRO GLY TYR THR ALA THR GLU ASP THR PHE LYS ASP THR ALA ASN LEU VAL LYS GLU ASP SER ASP VAL

• Molecule 3: unclear peptide

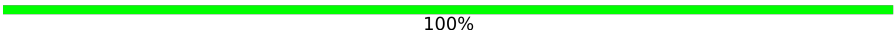
Chain G:



There are no outlier residues recorded for this chain.

• Molecule 4: unclear peptide

Chain H:



There are no outlier residues recorded for this chain.

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

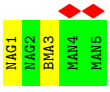
Chain D:

• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

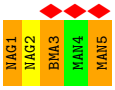
• Molecule 6: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:



• Molecule 7: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:


NAG1
NAG2
BMA3
MAN4
MAN5

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	67775	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.204	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.029	Depositor
Map size (Å)	366.86002, 366.86002, 366.86002	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.411, 1.411, 1.411	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, A2G, CA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	C	0.26	0/913	0.48	0/1220
2	A	0.30	0/9269	0.54	0/12573
2	B	0.29	0/1151	0.58	0/1569
4	H	0.21	0/7	0.40	0/8
All	All	0.29	0/11340	0.54	0/15370

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	895	0	885	17	0
2	A	9053	0	8306	126	0
2	B	1124	0	943	20	0
3	G	30	0	8	0	0
4	H	28	0	12	0	0
5	D	28	0	25	0	0
5	I	28	0	25	0	0
6	E	61	0	52	0	0
7	F	61	0	52	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	28	0	26	0	0
8	B	28	0	26	0	0
9	A	112	0	96	22	0
9	B	14	0	12	5	0
10	A	12	0	0	0	0
10	B	4	0	0	0	0
All	All	11506	0	10468	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:221:THR:OG1	9:A:4703:A2G:C1	1.68	1.39
2:B:2741:THR:HB	9:B:4703:A2G:C1	1.64	1.26
2:A:1271:THR:OG1	9:A:4709:A2G:C1	1.83	1.25
2:B:2741:THR:CB	9:B:4703:A2G:C1	2.23	1.15
2:B:2741:THR:HB	9:B:4703:A2G:O5	1.49	1.11
2:A:1065:THR:HB	9:A:4705:A2G:C1	1.81	1.10
2:A:1065:THR:CB	9:A:4705:A2G:C1	2.31	1.08
2:A:1149:THR:HB	9:A:4707:A2G:O5	1.55	1.07
2:A:1149:THR:CB	9:A:4707:A2G:C1	2.34	1.03
2:A:1149:THR:HB	9:A:4707:A2G:C1	1.87	1.02
2:A:1065:THR:OG1	9:A:4705:A2G:C1	2.13	0.97
2:B:2741:THR:OG1	9:B:4703:A2G:C1	2.18	0.91
2:A:221:THR:CB	9:A:4703:A2G:C1	2.53	0.86
2:A:1173:LYS:HD2	2:A:1178:GLY:HA2	1.61	0.81
2:A:1149:THR:OG1	9:A:4707:A2G:C1	2.29	0.80
2:A:1271:THR:HG21	9:A:4709:A2G:H3	1.67	0.76
2:B:2816:LYS:NZ	2:B:2832:THR:O	2.22	0.72
2:A:1271:THR:HG1	9:A:4709:A2G:C1	2.05	0.68
2:A:1065:THR:HB	9:A:4705:A2G:O5	1.93	0.67
1:C:291:ILE:O	1:C:295:ASN:ND2	2.29	0.65
2:A:281:ILE:HG21	2:A:330:PHE:CE2	2.31	0.65
2:A:912:MET:HE1	2:A:927:ILE:HG21	1.78	0.65
2:A:882:ARG:HE	2:A:895:HIS:HD2	1.45	0.64
2:A:281:ILE:HG21	2:A:330:PHE:HE2	1.61	0.64
1:C:281:ARG:HA	1:C:284:LEU:HD12	1.80	0.63
2:B:2741:THR:HB	9:B:4703:A2G:C5	2.27	0.63
2:B:2812:THR:HG23	2:B:2816:LYS:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1065:THR:HB	9:A:4705:A2G:C5	2.31	0.60
1:C:281:ARG:O	1:C:285:LYS:HG2	2.02	0.59
2:A:1065:THR:HG22	2:A:1066:CYS:O	2.02	0.59
2:A:1281:ASN:ND2	2:A:1297:CYS:O	2.32	0.59
2:A:1149:THR:HG22	2:A:1150:CYS:N	2.18	0.58
2:A:1272:CYS:SG	2:A:1276:HIS:HB2	2.43	0.58
2:A:295:ASP:OD1	2:A:304:ARG:NH2	2.36	0.58
2:A:616:THR:HG23	2:A:647:VAL:HG23	1.87	0.57
2:A:321:HIS:CD2	2:A:322:GLN:H	2.22	0.57
2:A:712:PHE:CE1	2:A:953:ILE:HD11	2.41	0.56
1:C:332:GLU:O	1:C:336:GLU:HG2	2.06	0.56
2:A:460:ILE:HD12	2:A:496:GLU:HA	1.88	0.55
2:A:738:SER:OG	2:A:739:PRO:HD3	2.07	0.55
1:C:324:LYS:O	1:C:328:VAL:HG22	2.08	0.53
2:A:371:LEU:H	2:A:371:LEU:HD23	1.72	0.53
2:A:247:CYS:C	2:A:249:ASP:H	2.11	0.53
2:A:569:ARG:NH2	2:A:589:GLN:O	2.40	0.53
2:A:486:LYS:HG2	2:A:736:THR:HG21	1.91	0.52
2:B:2801:CYS:N	2:B:2815:GLU:OE2	2.41	0.52
2:A:1126:ASP:OD2	2:A:1154:GLN:HG2	2.09	0.52
2:A:465:VAL:O	2:A:468:PRO:HD3	2.09	0.52
2:A:436:ARG:NH1	2:A:451:ASP:OD2	2.41	0.52
2:A:227:PHE:CZ	2:A:588:ILE:HD11	2.44	0.52
2:A:557:TRP:N	2:A:574:ASP:OD1	2.43	0.51
2:A:616:THR:HG23	2:A:647:VAL:CG2	2.40	0.51
2:A:311:CYS:HB2	2:A:327:GLY:HA3	1.92	0.51
1:C:271:ASN:ND2	2:A:725:LEU:HD22	2.24	0.51
2:A:484:GLU:OE1	2:A:486:LYS:N	2.43	0.51
2:B:2862:SER:O	2:B:2864:THR:N	2.43	0.51
2:A:1277:PHE:N	2:A:1285:ILE:O	2.40	0.50
2:A:358:ASP:O	2:A:359:GLN:HB2	2.12	0.50
2:A:818:ARG:NH1	2:A:1000:PRO:O	2.45	0.50
2:A:1065:THR:HG21	9:A:4705:A2G:HN2	1.76	0.49
2:A:197:LEU:HD22	2:A:197:LEU:H	1.77	0.49
2:A:316:CYS:HB2	2:A:343:ARG:O	2.12	0.49
2:A:1149:THR:HG22	2:A:1150:CYS:O	2.11	0.49
2:B:2759:TYR:HA	2:B:2762:ASP:OD1	2.12	0.49
2:A:1173:LYS:CD	2:A:1178:GLY:HA2	2.39	0.49
1:C:259:ARG:HH11	1:C:259:ARG:HG2	1.78	0.49
2:A:718:VAL:HB	2:A:735:VAL:HB	1.95	0.49
2:A:1281:ASN:OD1	2:A:1283:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:320:CYS:HA	2:A:329:CYS:HB2	1.95	0.48
2:A:321:HIS:HD2	2:A:322:GLN:HG2	1.78	0.48
2:A:1239:GLN:NE2	2:A:3180:CYS:O	2.40	0.48
2:A:321:HIS:HD2	2:A:322:GLN:H	1.61	0.48
2:A:447:VAL:O	2:A:460:ILE:N	2.42	0.48
2:A:735:VAL:HG11	2:A:756:TYR:CZ	2.49	0.48
2:A:357:CYS:HB3	2:A:370:CYS:HB3	1.75	0.47
2:A:953:ILE:HG23	2:A:956:VAL:HB	1.95	0.47
1:C:308:LEU:HD21	1:C:324:LYS:HZ2	1.78	0.47
2:A:221:THR:HB	9:A:4703:A2G:C1	2.42	0.47
2:A:221:THR:HB	9:A:4703:A2G:O5	2.14	0.47
2:B:2741:THR:HG22	2:B:2742:CYS:O	2.15	0.47
2:A:484:GLU:OE1	2:A:485:THR:N	2.49	0.46
2:A:494:ASN:OD1	2:A:495:LEU:N	2.48	0.46
2:A:725:LEU:O	2:A:725:LEU:HD23	2.15	0.46
2:A:244:ASP:OD1	2:A:245:ASP:N	2.48	0.46
2:A:321:HIS:CD2	2:A:322:GLN:HG2	2.51	0.46
2:A:215:ARG:HH11	2:A:216:ASN:HB2	1.81	0.46
2:A:538:GLU:HA	2:A:550:LEU:H	1.81	0.46
2:A:573:VAL:HG12	2:A:580:ILE:HG12	1.98	0.46
2:A:1151:GLN:HB2	2:A:1154:GLN:HG3	1.98	0.46
2:A:362:GLU:OE2	2:A:364:ARG:NE	2.49	0.46
2:A:865:ASN:HD22	7:F:1:NAG:C7	2.29	0.46
2:A:1065:THR:HG21	9:A:4705:A2G:N2	2.30	0.46
1:C:292:GLU:HA	1:C:295:ASN:HD21	1.82	0.45
2:A:318:TYR:HE2	2:A:330:PHE:HD1	1.64	0.45
2:A:371:LEU:HD23	2:A:371:LEU:N	2.31	0.45
2:A:999:CYS:SG	2:A:1005:LEU:HG	2.57	0.45
2:A:1151:GLN:N	2:A:1151:GLN:OE1	2.49	0.45
7:F:3:BMA:H5	7:F:5:MAN:H5	1.99	0.45
1:C:287:PHE:O	1:C:291:ILE:HG22	2.17	0.45
2:A:190:CYS:SG	2:A:191:GLY:N	2.90	0.45
2:A:364:ARG:O	2:A:367:ARG:HD3	2.17	0.45
1:C:293:LYS:NZ	2:A:203:ASP:OD2	2.46	0.45
2:A:1254:HIS:HD2	2:A:1256:ASP:OD1	1.99	0.45
2:A:580:ILE:HB	2:A:593:VAL:HG22	1.99	0.45
2:A:865:ASN:N	2:A:865:ASN:OD1	2.48	0.45
2:A:945:ASP:OD1	2:A:945:ASP:N	2.44	0.45
1:C:358:ASN:CB	2:A:725:LEU:HD21	2.47	0.44
2:A:422:ARG:HH21	2:A:1091:ASP:CG	2.20	0.44
2:B:2825:PRO:C	2:B:2827:PHE:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:188:PHE:O	2:A:196:ILE:N	2.50	0.44
2:A:1197:ASP:OD1	2:A:1199:SER:OG	2.33	0.44
2:A:461:LEU:HB3	2:A:465:VAL:HG21	2.00	0.44
2:A:788:LEU:HD23	2:A:799:TRP:HB3	2.00	0.44
2:A:1290:ILE:HG12	2:A:1306:CYS:SG	2.58	0.44
2:A:259:ASN:O	2:A:259:ASN:ND2	2.47	0.44
2:A:1149:THR:HB	9:A:4707:A2G:C5	2.47	0.44
2:A:882:ARG:HE	2:A:895:HIS:CD2	2.29	0.43
2:A:521:GLY:C	2:A:542:MET:HG3	2.39	0.43
1:C:316:ASP:HB3	1:C:319:HIS:HB2	1.99	0.43
2:A:221:THR:CB	9:A:4703:A2G:O5	2.67	0.43
2:A:624:MET:HE3	2:A:636:VAL:HA	2.01	0.43
2:B:2805:ASN:HB3	2:B:2808:HIS:CE1	2.53	0.43
2:A:221:THR:HG21	9:A:4703:A2G:O7	2.19	0.43
2:A:1050:CYS:C	2:A:1052:ASP:H	2.22	0.43
2:B:2797:LEU:O	2:B:2800:VAL:HG22	2.17	0.43
2:A:398:SER:HB3	2:A:645:HIS:O	2.18	0.43
1:C:358:ASN:HB2	2:A:725:LEU:HD21	2.01	0.43
2:A:621:MET:SD	2:A:1133:ASN:ND2	2.92	0.43
2:A:1173:LYS:HD2	2:A:1178:GLY:CA	2.41	0.43
2:A:896:SER:OG	2:A:901:LEU:O	2.23	0.42
2:A:3184:TYR:HD2	2:A:3195:GLN:HA	1.84	0.42
2:B:2795:ILE:HD13	2:B:2806:ASN:HB2	2.01	0.42
1:C:259:ARG:HG2	1:C:259:ARG:NH1	2.33	0.42
2:A:778:THR:HG23	2:A:782:LEU:HD11	2.02	0.42
2:A:1139:SER:HA	2:A:1142:LYS:HD3	2.01	0.42
2:A:1149:THR:HG21	9:A:4707:A2G:H3	2.01	0.42
2:A:1043:ARG:HA	2:A:1055:ASP:HB2	2.02	0.42
2:A:1066:CYS:HB3	2:A:1079:CYS:HB3	1.95	0.42
1:C:305:HIS:CE1	1:C:309:LYS:HE3	2.55	0.42
2:A:316:CYS:HB3	2:A:343:ARG:HA	2.02	0.42
2:A:471:LEU:HD11	2:A:480:LEU:HD21	2.02	0.42
2:A:280:SER:O	2:A:284:VAL:HG23	2.19	0.41
2:B:2786:GLU:O	2:B:2786:GLU:HG3	2.20	0.41
1:C:303:ILE:HD12	1:C:303:ILE:HA	1.86	0.41
2:A:1302:ASP:OD1	2:A:1302:ASP:N	2.48	0.41
2:B:2789:CYS:SG	2:B:2793:ARG:HB2	2.60	0.41
2:B:2806:ASN:H	2:B:2814:ASP:CG	2.24	0.41
2:A:361:CYS:SG	2:A:362:GLU:N	2.93	0.41
2:A:626:ALA:HB1	2:A:631:GLU:HG2	2.01	0.41
2:A:807:VAL:CG1	2:A:821:ILE:HB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2760:ARG:HD2	2:B:2772:ASP:O	2.21	0.41
2:A:1075:ARG:HD2	2:A:1094:ASP:HB2	2.02	0.41
2:A:555:VAL:HG12	2:A:558:PRO:HD3	2.03	0.41
2:A:840:PHE:CZ	2:A:898:LEU:HG	2.56	0.41
2:A:933:GLY:O	2:A:953:ILE:HG22	2.21	0.41
2:B:2800:VAL:HB	2:B:2817:ASN:HD21	1.85	0.41
2:A:1071:PHE:HE2	2:A:1085:HIS:CE1	2.39	0.41
2:A:212:SER:O	2:A:215:ARG:HG2	2.20	0.40
2:A:1062:PHE:CZ	2:A:1063:ASN:HB3	2.57	0.40
2:A:1175:CYS:N	2:A:1180:ASP:OD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	103/332 (31%)	103 (100%)	0	0	100	100
2	A	1163/4660 (25%)	1079 (93%)	83 (7%)	1 (0%)	51	82
2	B	146/4660 (3%)	131 (90%)	15 (10%)	0	100	100
4	H	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1413/9657 (15%)	1314 (93%)	98 (7%)	1 (0%)	54	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	359	GLN

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	99/299 (33%)	89 (90%)	10 (10%)	7 27
2	A	1026/4089 (25%)	989 (96%)	37 (4%)	35 63
2	B	132/4089 (3%)	125 (95%)	7 (5%)	22 52
4	H	1/1 (100%)	1 (100%)	0	100 100
All	All	1258/8478 (15%)	1204 (96%)	54 (4%)	33 59

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	259	ARG
1	C	268	GLN
1	C	290	LYS
1	C	305	HIS
1	C	307	LYS
1	C	323	ASN
1	C	324	LYS
1	C	327	TYR
1	C	342	LYS
1	C	346	GLN
2	A	198	ARG
2	A	215	ARG
2	A	221	THR
2	A	228	THR
2	A	268	ARG
2	A	310	VAL
2	A	311	CYS
2	A	321	HIS
2	A	329	CYS
2	A	330	PHE
2	A	348	PHE
2	A	350	ASP
2	A	429	ASP
2	A	436	ARG

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Mol	Chain	Res	Type
2	A	470	ASN
2	A	489	ARG
2	A	516	LEU
2	A	527	ASP
2	A	550	LEU
2	A	593	VAL
2	A	631	GLU
2	A	681	ASN
2	A	711	LEU
2	A	746	ASP
2	A	807	VAL
2	A	887	ASP
2	A	950	ARG
2	A	992	ASN
2	A	995	ARG
2	A	1010	MET
2	A	1018	ARG
2	A	1071	PHE
2	A	1093	LEU
2	A	1114	SER
2	A	1173	LYS
2	A	1180	ASP
2	A	1230	MET
2	B	2718	TRP
2	B	2731	ASP
2	B	2753	ARG
2	B	2786	GLU
2	B	2815	GLU
2	B	2837	VAL
2	B	2839	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	295	ASN
1	C	323	ASN
2	A	321	HIS
2	A	382	GLN
2	A	412	ASN
2	A	444	GLN
2	A	456	ASN
2	A	639	GLN

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Mol	Chain	Res	Type
2	A	681	ASN
2	A	895	HIS
2	A	978	HIS
2	A	992	ASN
2	A	1058	GLN
2	A	1099	GLN
2	A	1160	HIS
2	A	1254	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

14 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	D	1	5,2	14,14,15	0.41	0	17,19,21	1.86	2 (11%)
5	NAG	D	2	5	14,14,15	0.31	0	17,19,21	0.81	1 (5%)
6	NAG	E	1	6,2	14,14,15	0.32	0	17,19,21	0.85	1 (5%)
6	NAG	E	2	6	14,14,15	0.30	0	17,19,21	0.62	0
6	BMA	E	3	6	11,11,12	0.28	0	15,15,17	0.94	1 (6%)
6	MAN	E	4	6	11,11,12	0.23	0	15,15,17	0.73	0
6	MAN	E	5	6	11,11,12	0.28	0	15,15,17	0.78	0
7	NAG	F	1	7,2	14,14,15	0.33	0	17,19,21	0.74	1 (5%)
7	NAG	F	2	7	14,14,15	0.44	0	17,19,21	1.73	5 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BMA	F	3	7	11,11,12	0.38	0	15,15,17	1.73	2 (13%)
7	MAN	F	4	7	11,11,12	0.27	0	15,15,17	0.74	0
7	MAN	F	5	7	11,11,12	0.40	0	15,15,17	1.10	2 (13%)
5	NAG	I	1	5,2	14,14,15	0.50	0	17,19,21	1.67	5 (29%)
5	NAG	I	2	5	14,14,15	0.37	0	17,19,21	1.30	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	D	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	D	2	5	-	0/6/23/26	0/1/1/1
6	NAG	E	1	6,2	-	0/6/23/26	0/1/1/1
6	NAG	E	2	6	-	0/6/23/26	0/1/1/1
6	BMA	E	3	6	-	0/2/19/22	0/1/1/1
6	MAN	E	4	6	-	0/2/19/22	0/1/1/1
6	MAN	E	5	6	-	0/2/19/22	0/1/1/1
7	NAG	F	1	7,2	-	0/6/23/26	0/1/1/1
7	NAG	F	2	7	-	4/6/23/26	0/1/1/1
7	BMA	F	3	7	-	1/2/19/22	0/1/1/1
7	MAN	F	4	7	-	0/2/19/22	0/1/1/1
7	MAN	F	5	7	-	1/2/19/22	0/1/1/1
5	NAG	I	1	5,2	-	4/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1	NAG	C1-O5-C5	6.58	121.11	112.19
5	I	2	NAG	C1-O5-C5	4.37	118.12	112.19
7	F	2	NAG	C3-C4-C5	4.36	118.01	110.24
7	F	3	BMA	O5-C5-C6	4.24	113.85	107.20
5	I	1	NAG	O5-C1-C2	-4.10	104.82	111.29
7	F	3	BMA	C1-O5-C5	-3.47	107.50	112.19
7	F	2	NAG	C4-C3-C2	2.78	115.09	111.02
7	F	5	MAN	C1-O5-C5	2.67	115.81	112.19
7	F	2	NAG	O5-C1-C2	-2.53	107.29	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	2	NAG	O3-C3-C2	-2.50	104.29	109.47
5	I	1	NAG	C4-C3-C2	-2.43	107.46	111.02
5	D	2	NAG	C1-O5-C5	2.42	115.47	112.19
6	E	3	BMA	C1-C2-C3	2.38	112.59	109.67
6	E	1	NAG	C1-O5-C5	2.37	115.40	112.19
7	F	5	MAN	C1-C2-C3	2.35	112.55	109.67
7	F	2	NAG	C2-N2-C7	-2.22	119.74	122.90
5	I	1	NAG	O5-C5-C4	2.21	116.21	110.83
5	I	1	NAG	C6-C5-C4	-2.21	107.83	113.00
5	D	1	NAG	O5-C1-C2	-2.13	107.92	111.29
7	F	1	NAG	O5-C1-C2	-2.06	108.03	111.29
5	I	1	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	2	NAG	O5-C5-C6-O6
7	F	3	BMA	O5-C5-C6-O6
7	F	2	NAG	C8-C7-N2-C2
7	F	2	NAG	C4-C5-C6-O6
7	F	2	NAG	O7-C7-N2-C2
5	I	1	NAG	C8-C7-N2-C2
7	F	5	MAN	O5-C5-C6-O6
5	I	1	NAG	O7-C7-N2-C2
5	I	2	NAG	C1-C2-N2-C7
5	I	1	NAG	C1-C2-N2-C7
5	I	1	NAG	C3-C2-N2-C7

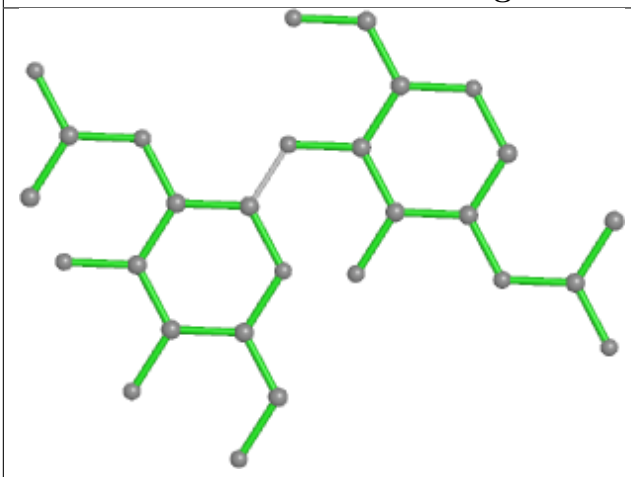
There are no ring outliers.

3 monomers are involved in 2 short contacts:

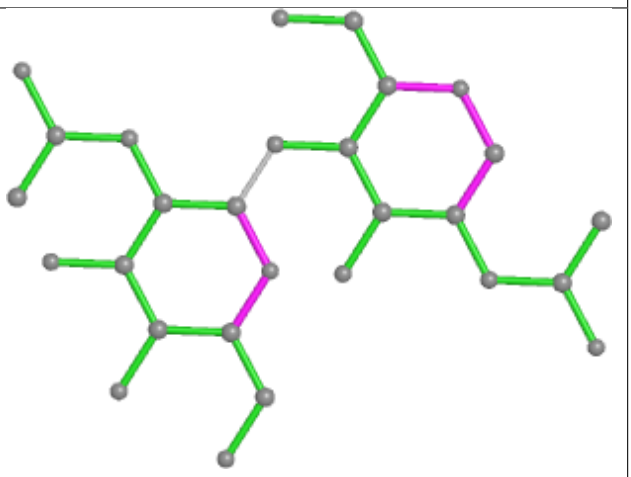
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	5	MAN	1	0
7	F	1	NAG	1	0
7	F	3	BMA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

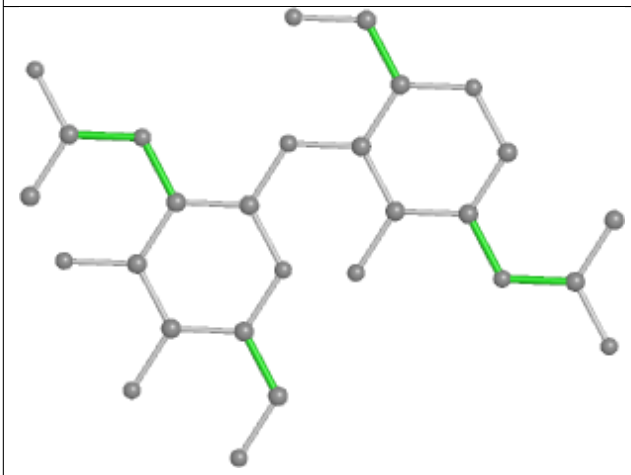
Oligosaccharide Chain D



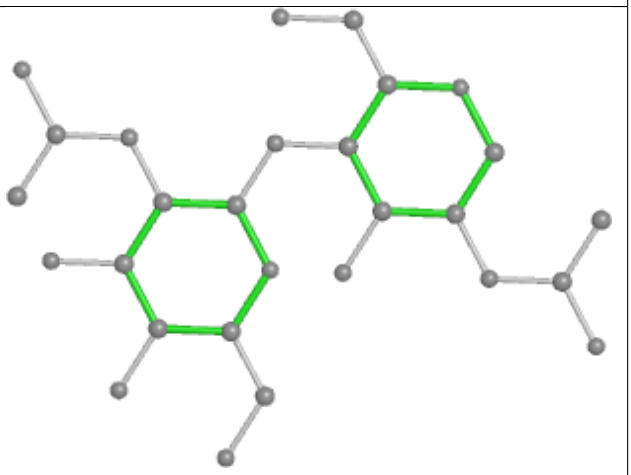
Bond lengths



Bond angles

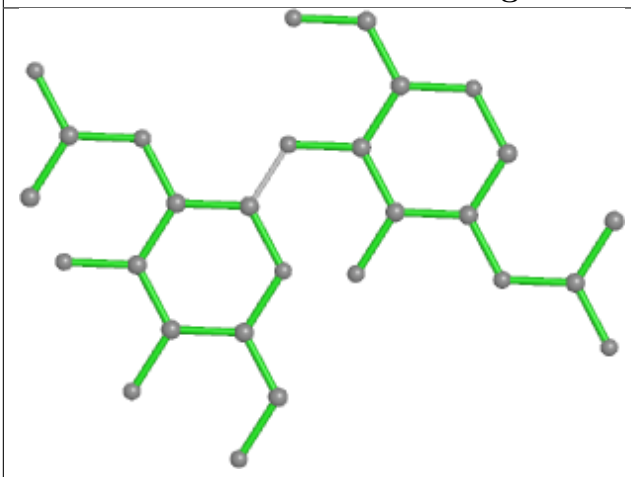


Torsions

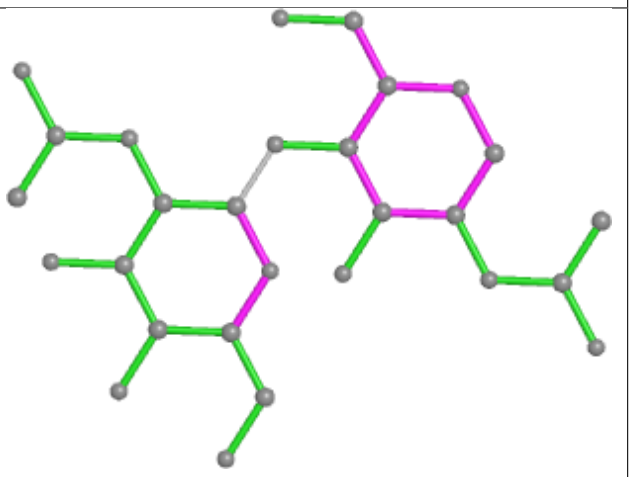


Rings

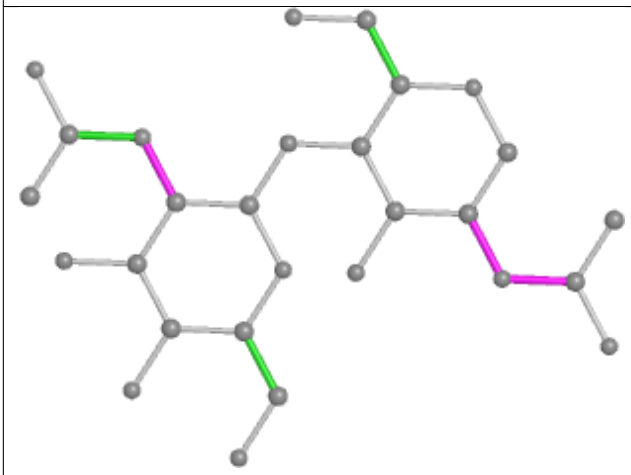
Oligosaccharide Chain I



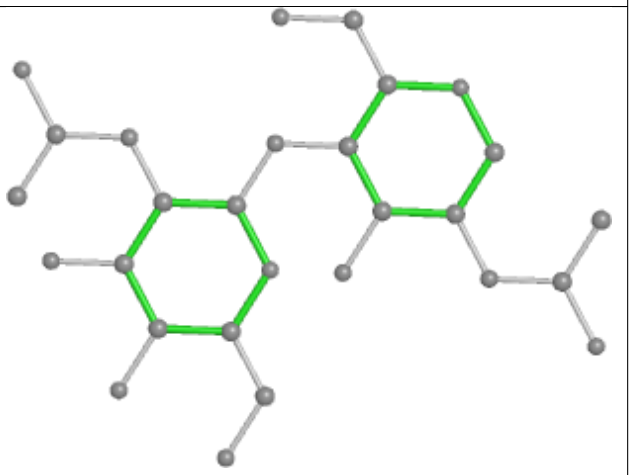
Bond lengths



Bond angles

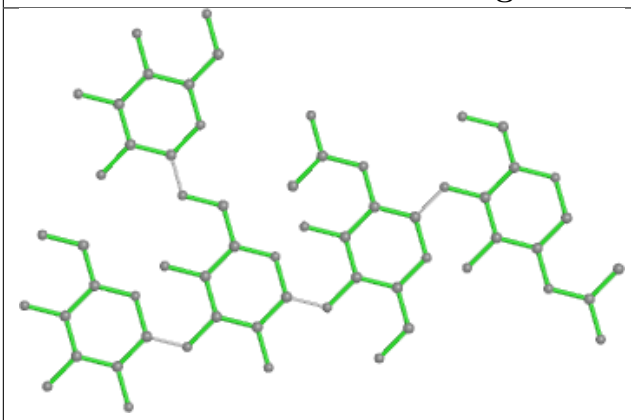


Torsions

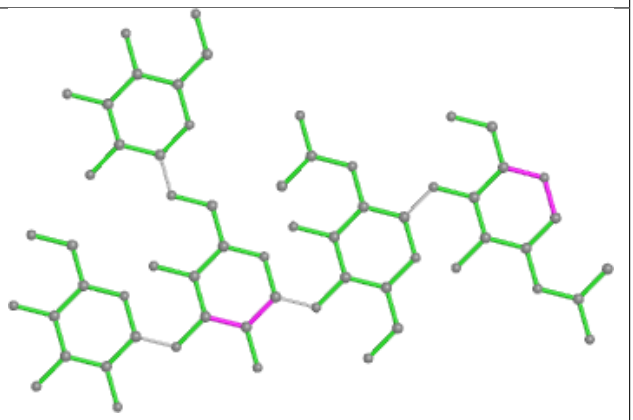


Rings

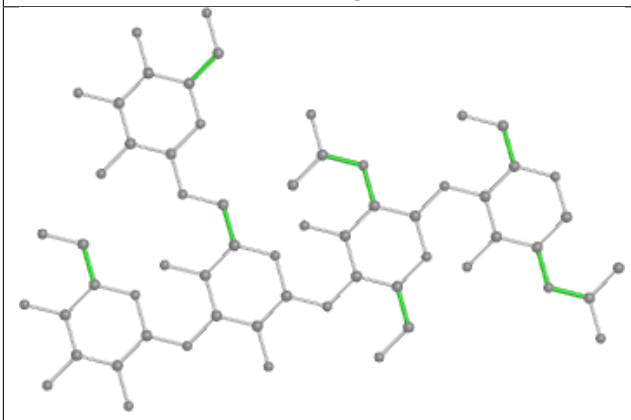
Oligosaccharide Chain E



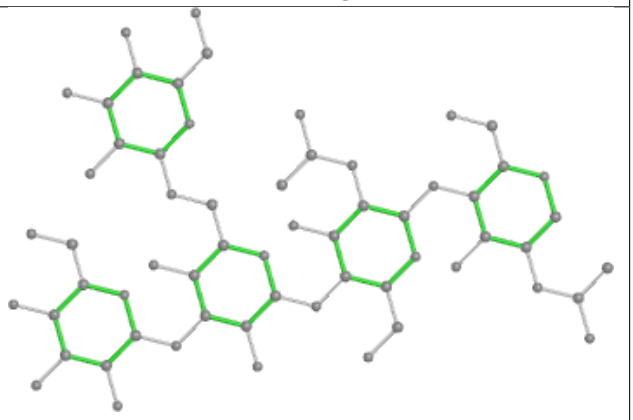
Bond lengths



Bond angles

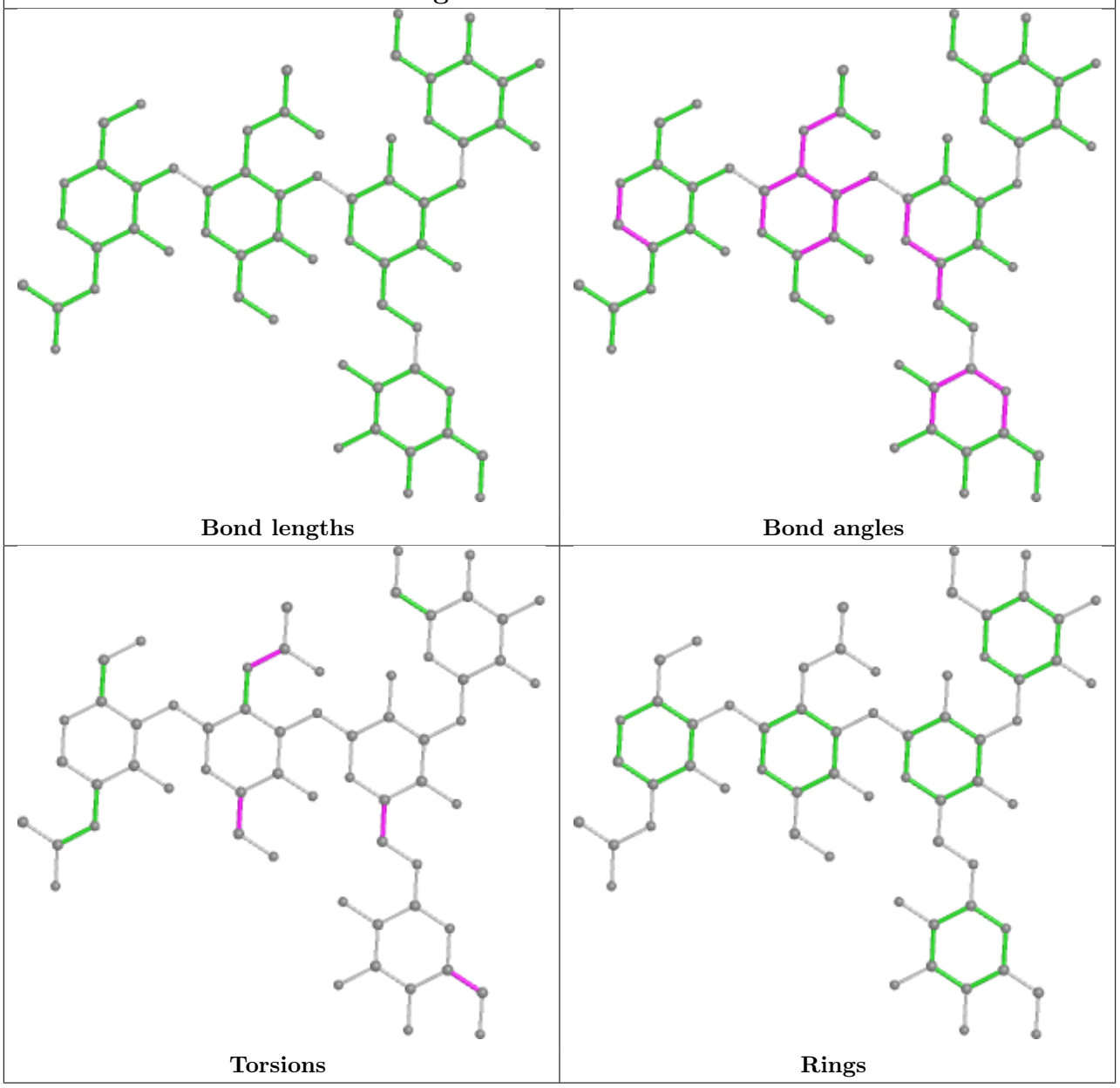


Torsions



Rings

Oligosaccharide Chain F



5.6 Ligand geometry (i)

Of 29 ligands modelled in this entry, 16 are monoatomic - leaving 13 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	NAG	A	4702	2	14,14,15	0.44	0	17,19,21	2.06	1 (5%)
8	NAG	A	4701	2	14,14,15	0.29	0	17,19,21	1.17	2 (11%)
9	A2G	A	4707	-	14,14,15	0.40	0	17,19,21	2.57	3 (17%)
9	A2G	A	4708	2	14,14,15	0.40	0	17,19,21	1.01	1 (5%)
9	A2G	A	4709	-	14,14,15	0.38	0	17,19,21	1.84	3 (17%)
9	A2G	A	4710	2	14,14,15	0.37	0	17,19,21	1.32	2 (11%)
9	A2G	A	4706	2	14,14,15	0.39	0	17,19,21	0.80	1 (5%)
9	A2G	B	4703	-	14,14,15	0.42	0	17,19,21	2.40	3 (17%)
9	A2G	A	4705	-	14,14,15	0.44	0	17,19,21	2.44	3 (17%)
9	A2G	A	4703	-	14,14,15	0.42	0	17,19,21	2.36	4 (23%)
8	NAG	B	4702	2	14,14,15	0.51	0	17,19,21	2.68	4 (23%)
8	NAG	B	4701	2	14,14,15	0.32	0	17,19,21	0.63	0
9	A2G	A	4704	2	14,14,15	0.43	0	17,19,21	0.67	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	NAG	A	4702	2	-	0/6/23/26	0/1/1/1
8	NAG	A	4701	2	-	0/6/23/26	0/1/1/1
9	A2G	A	4707	-	-	2/6/23/26	0/1/1/1
9	A2G	A	4708	2	-	0/6/23/26	0/1/1/1
9	A2G	A	4709	-	-	1/6/23/26	0/1/1/1
9	A2G	A	4710	2	-	0/6/23/26	0/1/1/1
9	A2G	A	4706	2	-	0/6/23/26	0/1/1/1
9	A2G	B	4703	-	-	0/6/23/26	0/1/1/1
9	A2G	A	4705	-	-	3/6/23/26	0/1/1/1
9	A2G	A	4703	-	-	1/6/23/26	0/1/1/1
8	NAG	B	4702	2	-	2/6/23/26	0/1/1/1
8	NAG	B	4701	2	-	0/6/23/26	0/1/1/1
9	A2G	A	4704	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	B	4703	A2G	O5-C1-C2	8.86	125.27	111.29
8	B	4702	NAG	C1-O5-C5	8.80	124.11	112.19
9	A	4705	A2G	O5-C1-C2	8.36	124.48	111.29
8	A	4702	NAG	C1-O5-C5	8.13	123.20	112.19
9	A	4703	A2G	O5-C1-C2	7.92	123.79	111.29
9	A	4707	A2G	O5-C1-C2	7.89	123.75	111.29
9	A	4709	A2G	C2-N2-C7	6.36	131.96	122.90
9	A	4707	A2G	C2-N2-C7	5.66	130.96	122.90
9	A	4710	A2G	O5-C1-C2	-4.53	104.14	111.29
8	B	4702	NAG	C4-C3-C2	-4.15	104.94	111.02
9	A	4705	A2G	C1-C2-N2	4.10	117.48	110.49
9	A	4707	A2G	C1-O5-C5	3.89	117.46	112.19
9	A	4708	A2G	O5-C1-C2	3.75	117.21	111.29
9	A	4705	A2G	C1-O5-C5	3.64	117.13	112.19
9	A	4703	A2G	C1-C2-N2	3.53	116.51	110.49
8	A	4701	NAG	C1-O5-C5	3.46	116.88	112.19
9	B	4703	A2G	C1-O5-C5	3.39	116.79	112.19
9	A	4709	A2G	O5-C1-C2	3.27	116.45	111.29
9	A	4703	A2G	C2-N2-C7	3.24	127.51	122.90
8	B	4702	NAG	C2-N2-C7	-3.23	118.30	122.90
8	B	4702	NAG	C6-C5-C4	-2.99	105.99	113.00
9	A	4703	A2G	C1-O5-C5	2.88	116.09	112.19
9	A	4710	A2G	C1-C2-N2	2.80	115.26	110.49
9	B	4703	A2G	C1-C2-N2	2.44	114.65	110.49
9	A	4709	A2G	C1-O5-C5	2.35	115.38	112.19
9	A	4706	A2G	C1-C2-N2	2.33	114.46	110.49
9	A	4704	A2G	C1-C2-N2	2.22	114.28	110.49
8	A	4701	NAG	C4-C3-C2	-2.10	107.94	111.02

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	4707	A2G	C3-C2-N2-C7
9	A	4709	A2G	C3-C2-N2-C7
9	A	4705	A2G	O5-C5-C6-O6
9	A	4707	A2G	O5-C5-C6-O6
8	B	4702	NAG	C8-C7-N2-C2
8	B	4702	NAG	O7-C7-N2-C2
9	A	4705	A2G	C1-C2-N2-C7
9	A	4703	A2G	C3-C2-N2-C7
9	A	4705	A2G	C3-C2-N2-C7

There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	4707	A2G	6	0
9	A	4709	A2G	3	0
9	B	4703	A2G	5	0
9	A	4705	A2G	7	0
9	A	4703	A2G	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

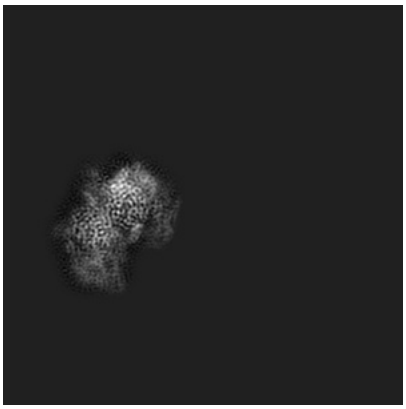
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36702. These allow visual inspection of the internal detail of the map and identification of artifacts.

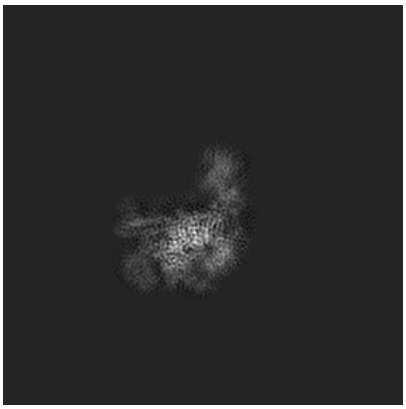
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

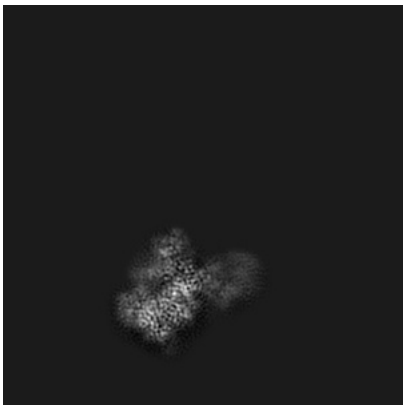
6.1.1 Primary map



X

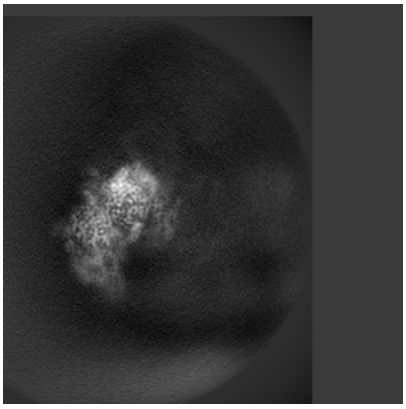


Y

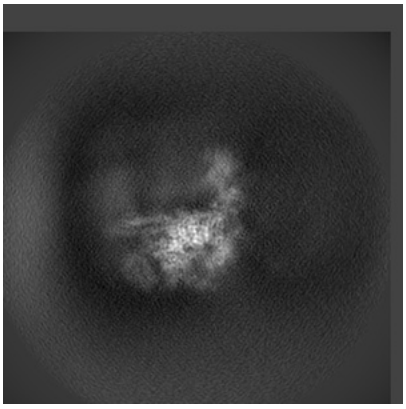


Z

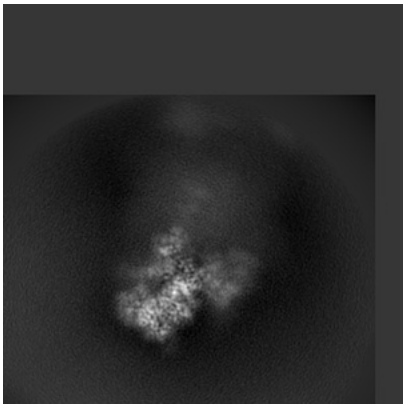
6.1.2 Raw map



X



Y

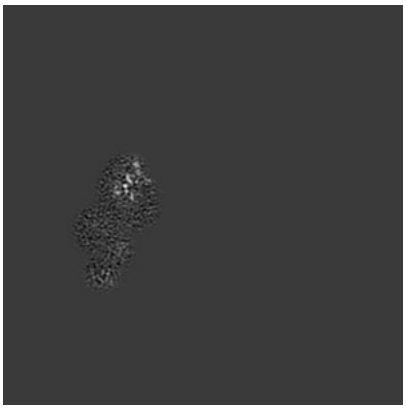


Z

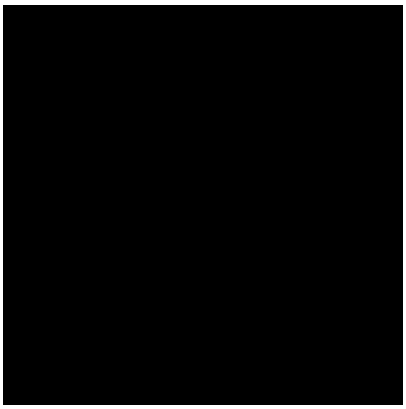
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



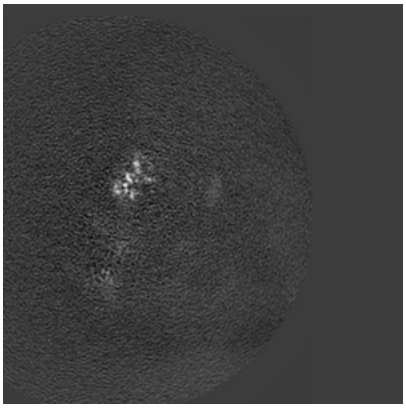
X Index: 130



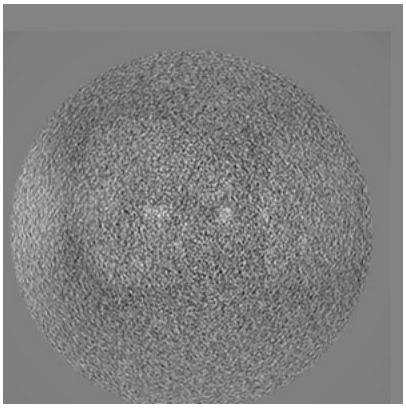
Y Index: 130

Z Index: 130

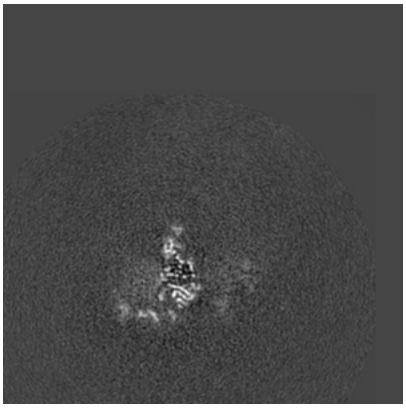
6.2.2 Raw map



X Index: 130



Y Index: 130

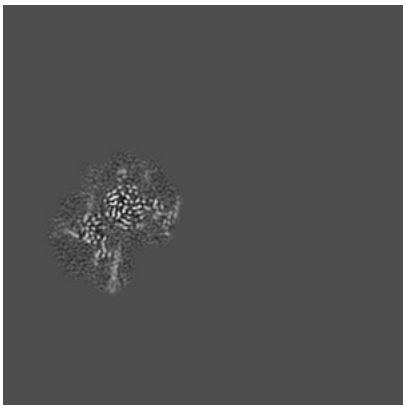


Z Index: 130

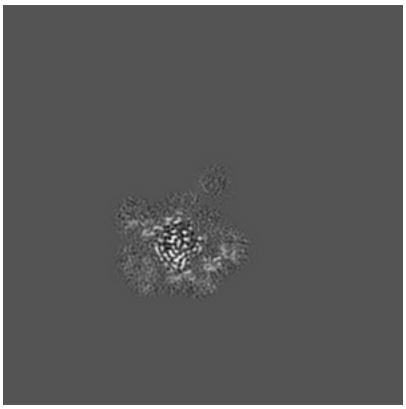
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



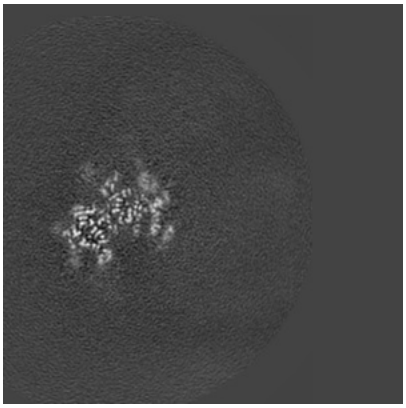
X Index: 111



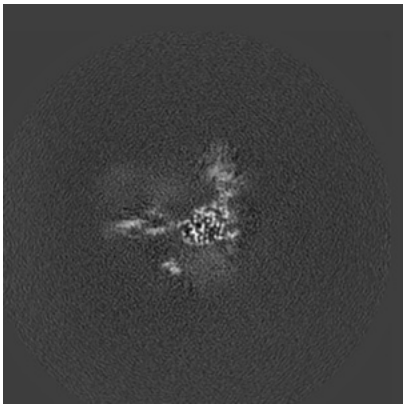
Y Index: 60

Z Index: 117

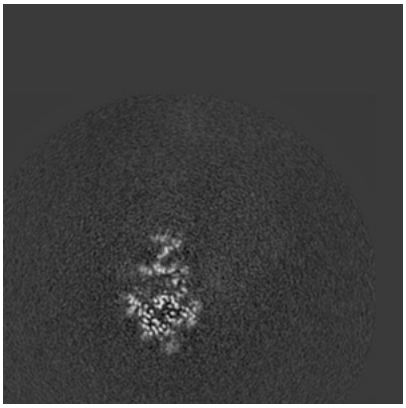
6.3.2 Raw map



X Index: 105



Y Index: 75

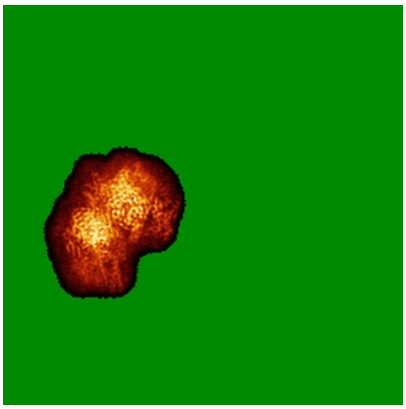


Z Index: 115

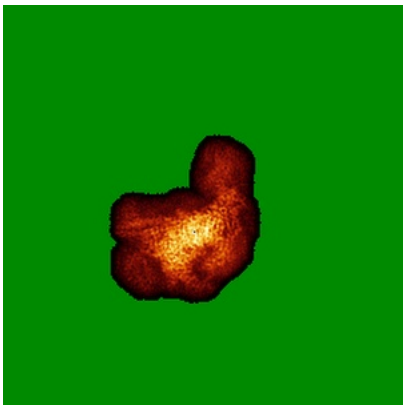
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

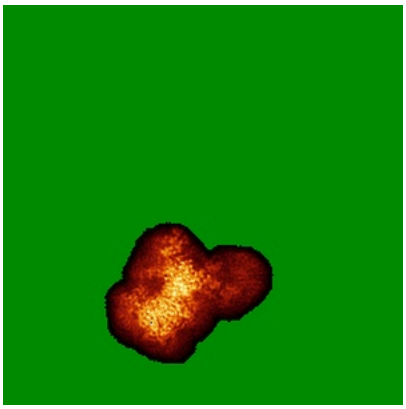
6.4.1 Primary map



X

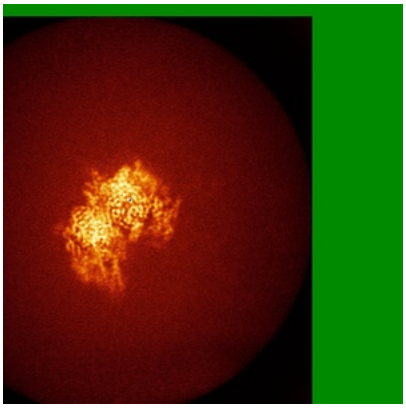


Y

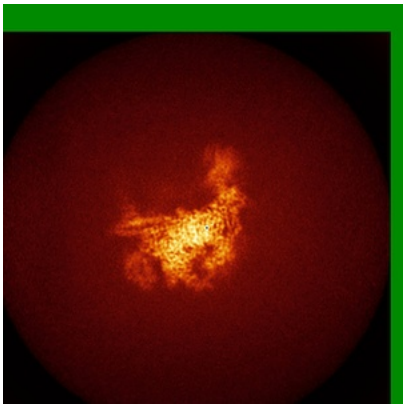


Z

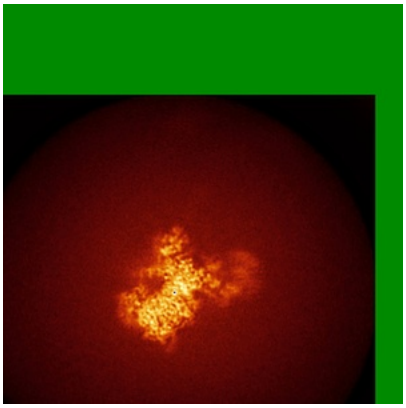
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.029. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

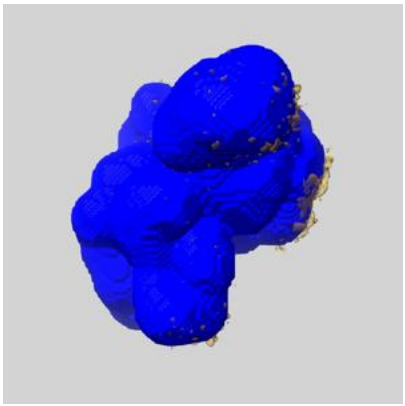
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

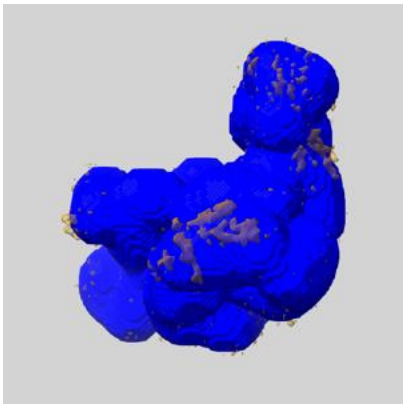
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

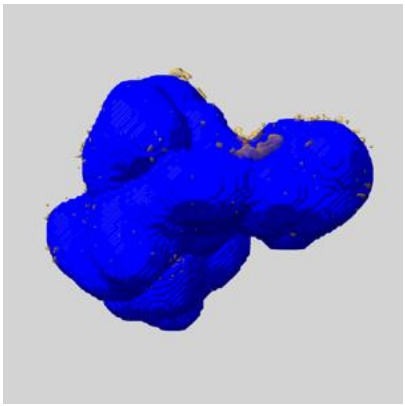
6.6.1 emd_36702_msk_1.map (i)



X



Y

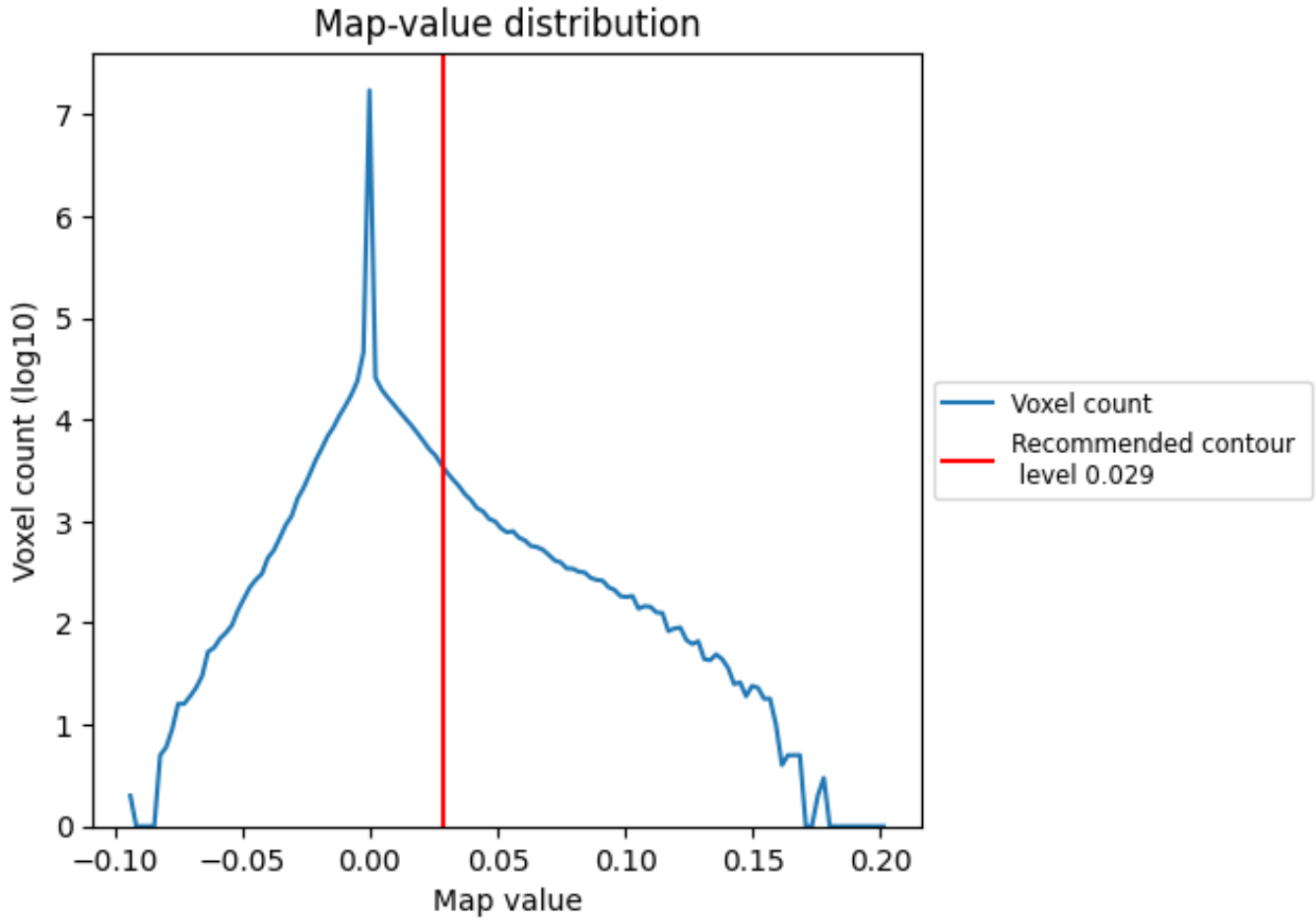


Z

7 Map analysis

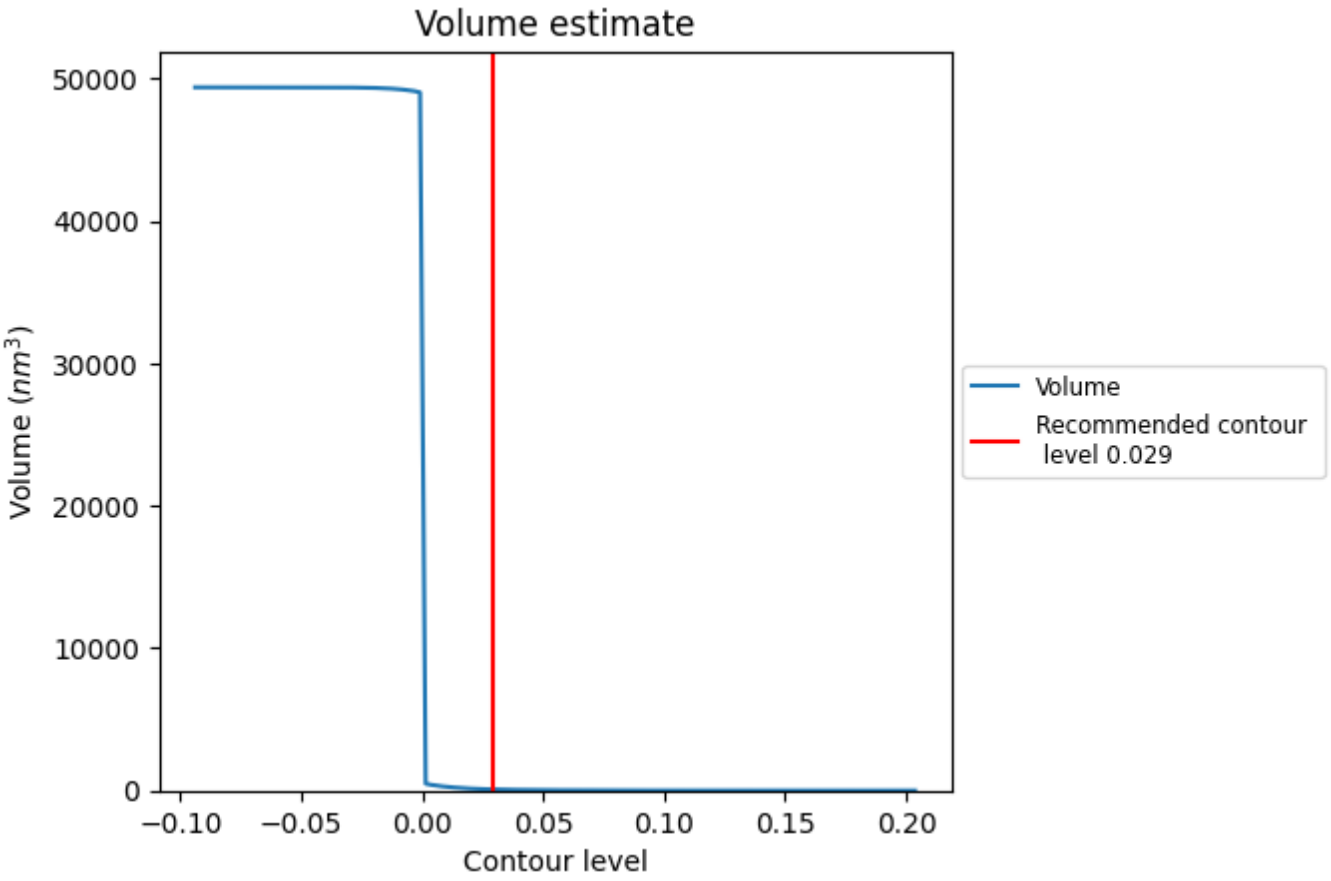
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

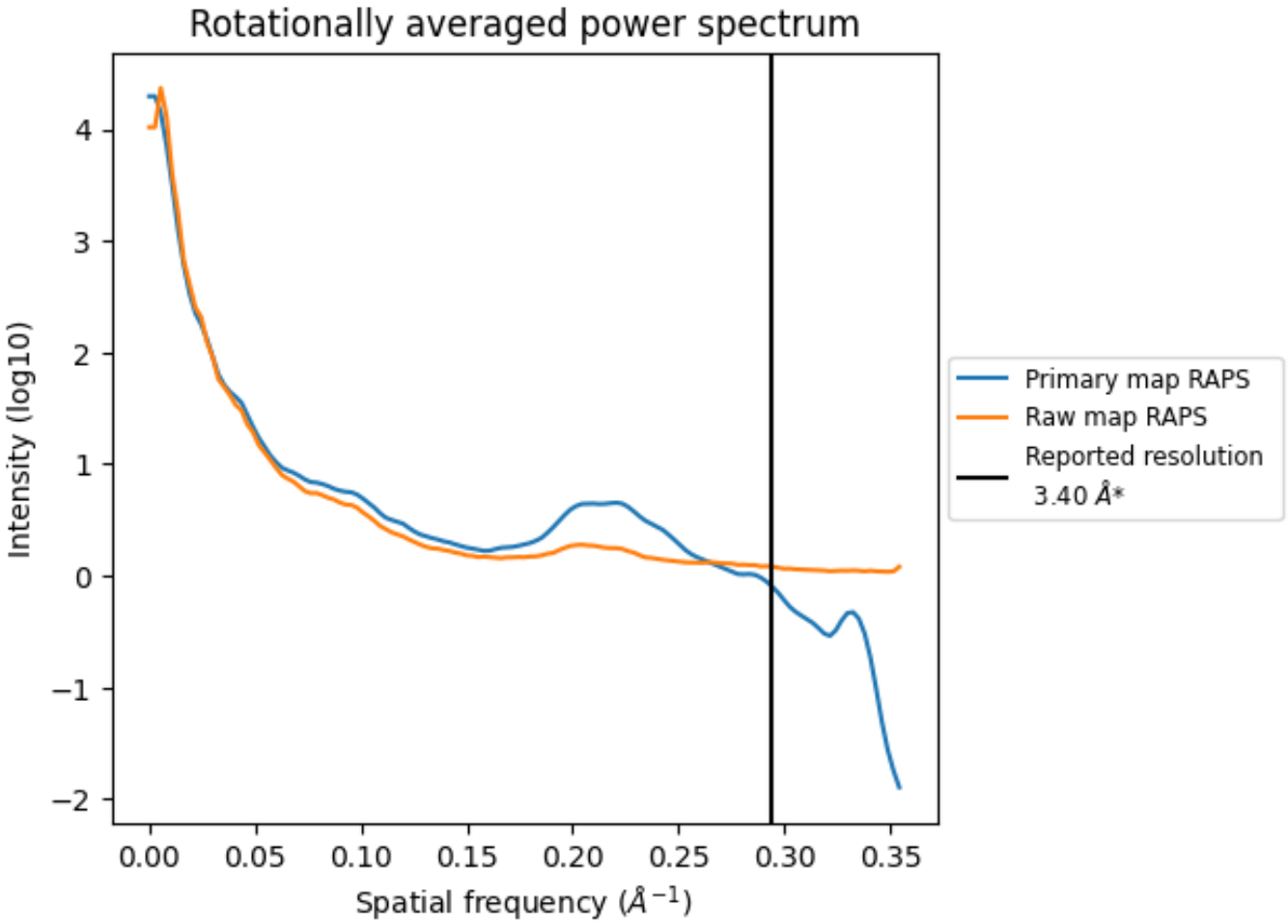
7.2 Volume estimate



The volume at the recommended contour level is 82 nm^3; this corresponds to an approximate mass of 74 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

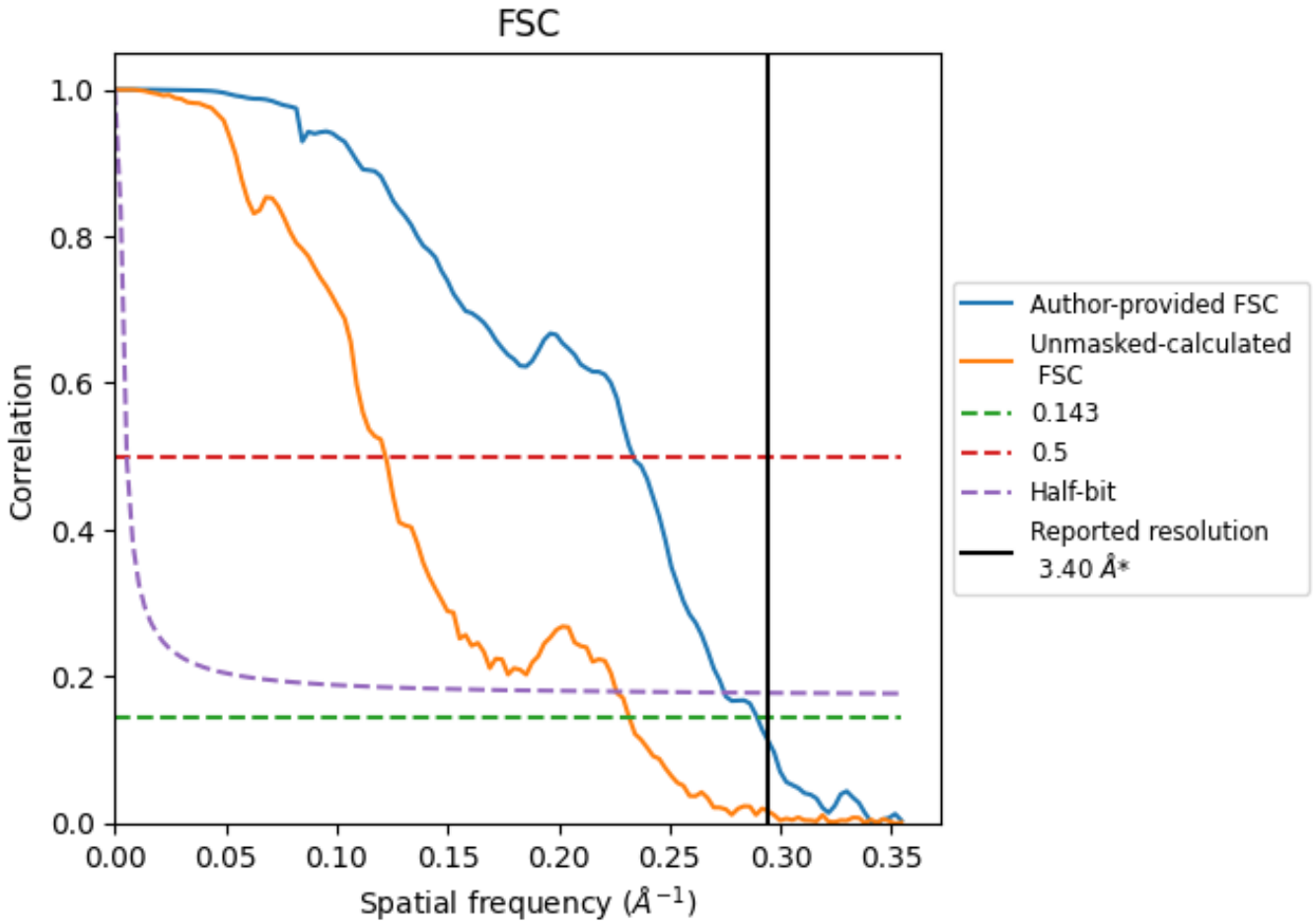


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

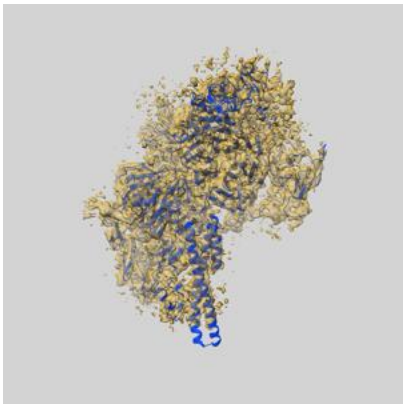
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.45	4.28	3.64
Unmasked-calculated*	4.31	8.20	4.42

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.31 differs from the reported value 3.4 by more than 10 %

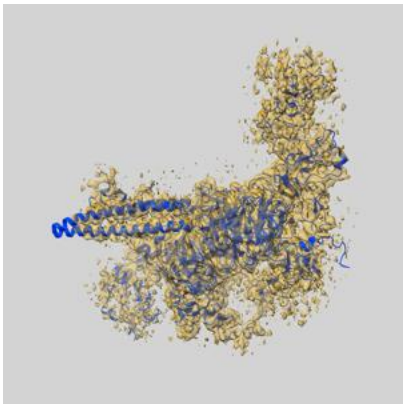
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36702 and PDB model 8JXI. Per-residue inclusion information can be found in section 3 on page 8.

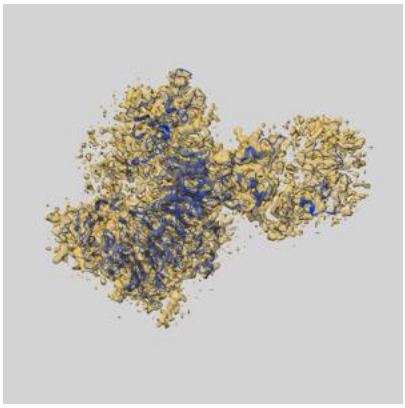
9.1 Map-model overlay



X



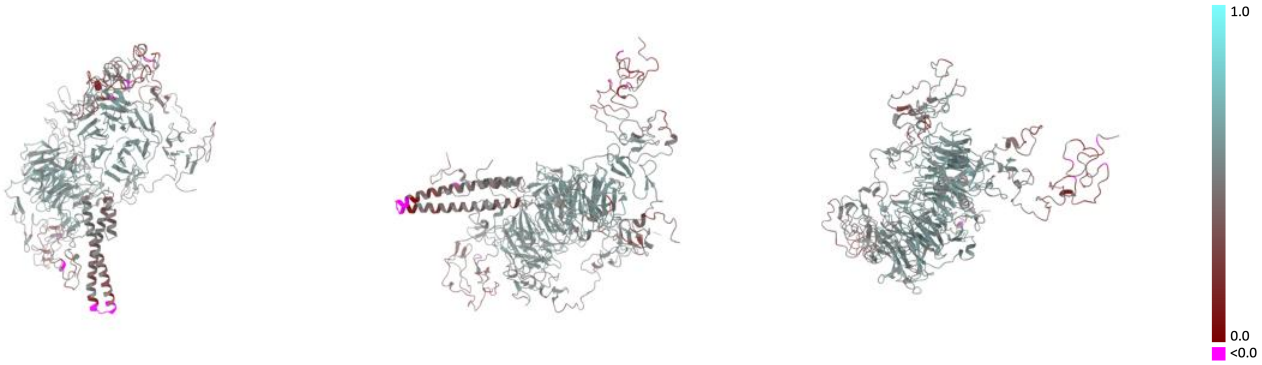
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

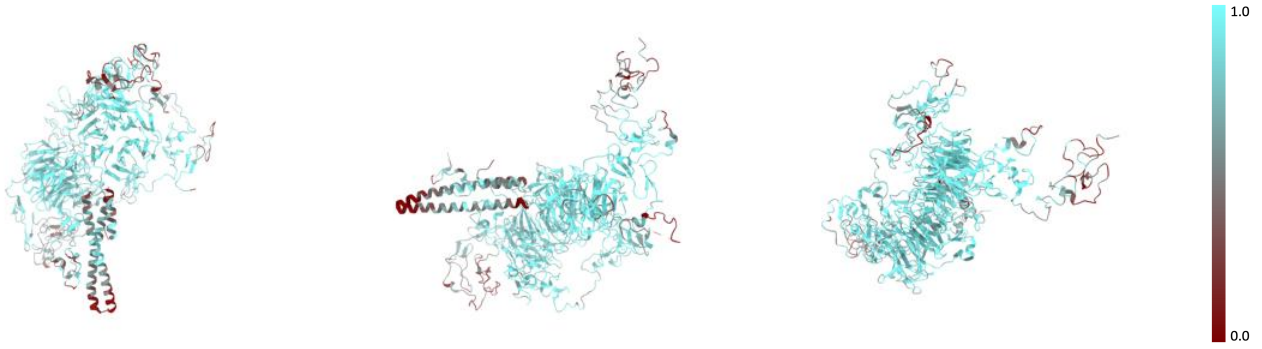
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

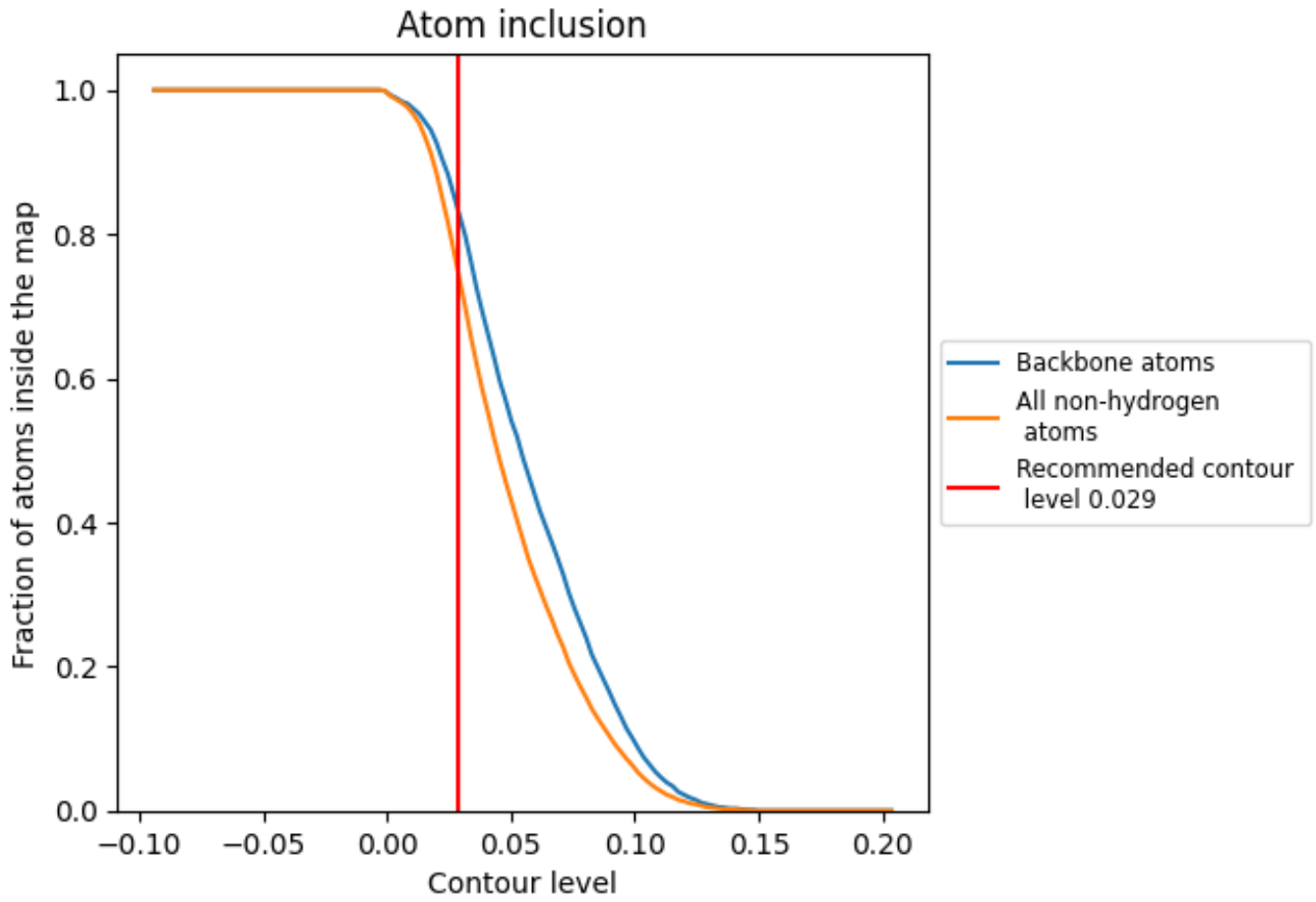
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.029).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7430	0.4790
A	0.7920	0.5070
B	0.5900	0.3530
C	0.4830	0.3660
D	0.5000	0.4690
E	0.5080	0.4280
F	0.4750	0.4020
G	0.9000	0.5370
H	0.9640	0.5780
I	0.3570	0.2720